2nd Workshop on Neutron Cross Section Covariances
Vienna University of Technology, Atominstitut

Importance of Nuclear Data Uncertainties in Criticality Calculations

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September 14 -16 2011

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1. What's UAM?

Organization for Economic Co-operation and Development (OECD) / Nuclear Energy Agency (NEA) / Nuclear Science Committee (NSC) has approved the birth of an

Expert Group on Uncertainty Analysis in Modeling (UAM).

↓

Benchmark for **Uncertainty Analysis in Modeling** for Design, Operation, and Safety Analysis of Light Water Reactor

(OECD LWR UAM benchmark)

2. “Cell Physics” Benchmark: Exercise I-1

To study the propagation of the uncertainty from basic data across different scale and physics phenomena → through complex coupled multi-physics and multi-scale simulations (see Ref.).

Benchmark’s structure

Phase I (Neutronics Phase)

- **Exercise 1 (I-1):“Cell Physics” focused on the derivation of the multi-group microscopic cross-section libraries (PWR**, BWR, VVER, GENIV …**)**
- Exercise 2 (I-2):“Lattice Physics” focused on the derivation of the few-group macroscopic cross-section libraries.
- Exercise 3 (I-3): “Core Physics” focused on the core steady state stand-alone neutronics calculations

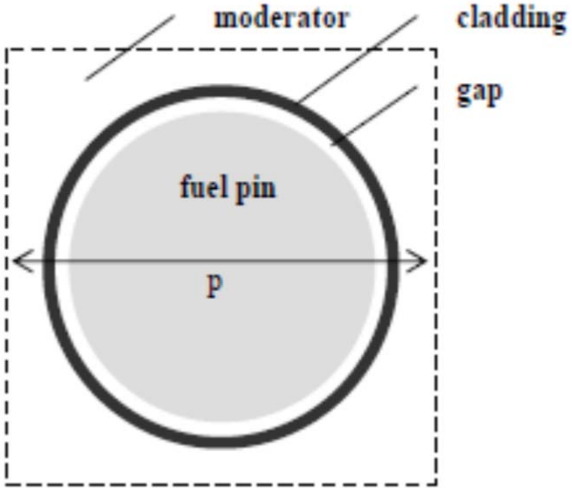
Phase II (Core Phase)

Phase III (System Phase)

Ref. “Verification, validation and uncertainty quantification in multi-physics modeling for nuclear reactor design and safety analysis”, Maria N. Avramova, Kostadin N. Ivanov, Progress in Nuclear Energy 52 (2010) 601-614

Exercise I-1: Problem description

PWR (TMI-1)



p – pitch of the unit cell

4.85%wt in U235

HFP Conditions / Reactor	PB-2 BWR	TMI-1 PWR
Fuel Temperature, [K]	900	900
Cladding Temperature, [K]	600	600
Moderator (Coolant) Temperature, [K]	557	562
Moderator (Coolant) Density, [kg/m^3]	743.6	748.4
Reactor Power, [MWt]	3293	2772

HZP Conditions / Reactor	PB-2 BWR	TMI-1 PWR
Fuel Temperature, [K]	552.833	551.000
Moderator (Coolant) Temperature, [K]	552.833	551.000
Moderator (Coolant) Density, [kg/m^3]	753.978	766.000
Reactor Power ,[MWt]	3.293	2.772

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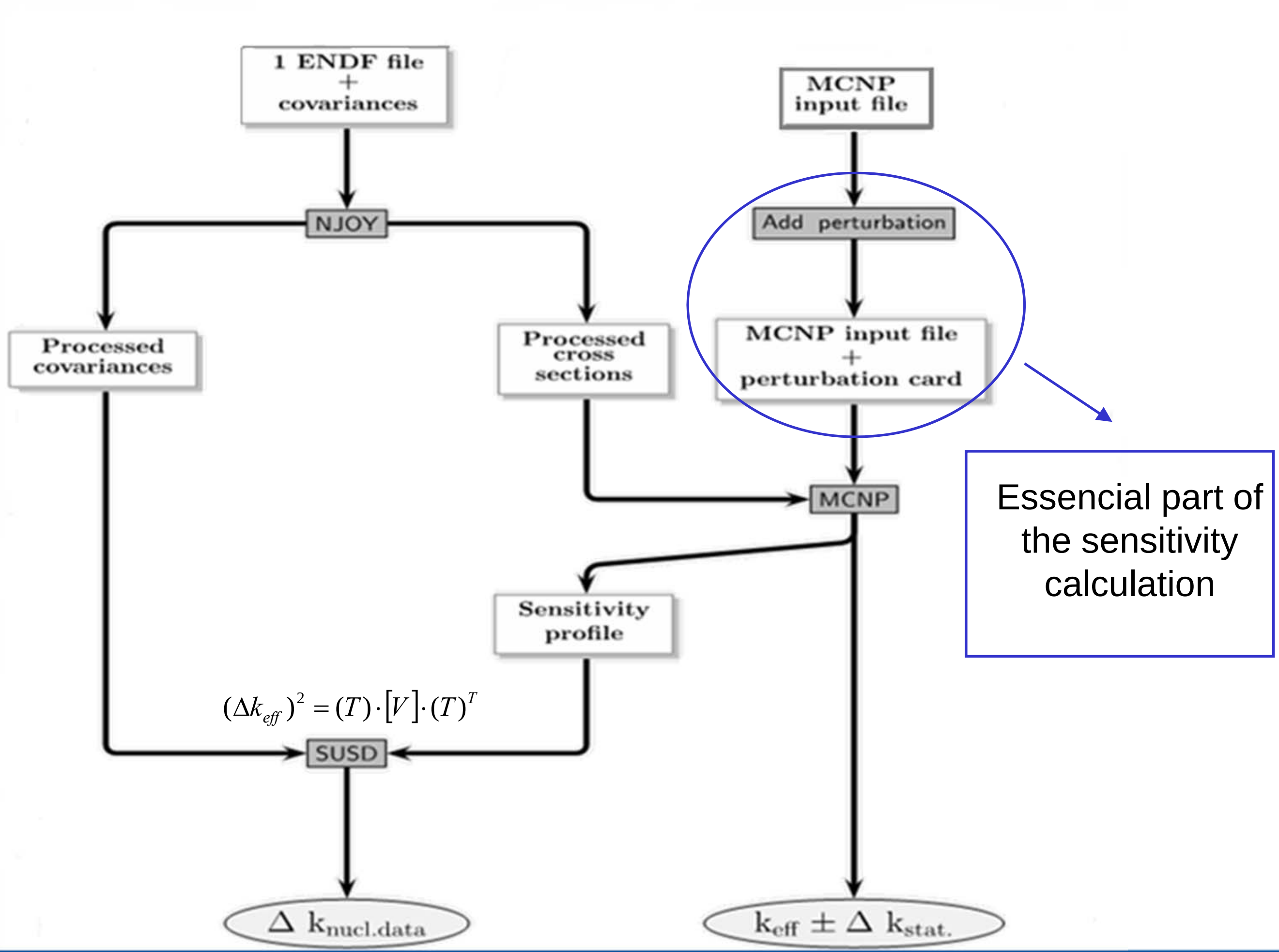
Exercise I-1: Participants

University/ research centre	Codes/libraries
UPM (Spain)	**MCNP5/SCALE6.0**
UPC (Spain)	SCALE 6.0/ Tsunami
Pisa (Italia)	DRAGON with library WIMS Based on ENDF/B VII JEFF-3.1 JENDL-3.2
AEKI (Hungría)	Multicell code a part of KARATE Based on ENDF/B VII
PSI (Suiza)	CASMO-5
Grenoble (Francia)	DRAGON and SUSD3D
VTT (Finlandia)	CASMO-4/TSUNAMI Based on ENDF/B VII
JNES Japan	CASMO-4 Based on JENDL-3.3

3. UPM Methodology: Exercise I-1

The perturbation approach relies in principle on a unique “**NJOY + MCNP5 + SUSD3D**” calculation. The inputs are the geometry MCNP5 input file and an ENDF file containing covariances.

- ENDF file, ENDF/B-VII, is processed by NJOY at different temperatures in ACE format. Ref: ***T. Viitanen and J. Leppänen,, NEA-1854 ZZ-SERPENT117 - ACELIB***
- ENDF Covariances can be processed with NJOY (used by SUSD3D).
- ANGELO, LAMDA and NJOY codes are used to generate processed covariances in 44g to SUSD3D code
- Sensitivity profiles (elastic, inelastic, capture, fission and 2,2n) are processed to SUSD3 code



MCNP5 PERT card

To compute sensitivities coefficients we used the **PERT card** of MCNP5.

The PERT-card is created specifying that the relevant material is replaced by the perturbated material in each of the cells in wich the material is present.

Perturbation cards are given for all energy groups (44). At the end we have **880 PERT-cards:** (4 isotopes X 5reactions X 44 groups).

Indicates wich cells are parturbated.

Specifies the perturbacion material number.

Specifies the perturbeted density of the cell.

```
PERT1:N   CELL=10  MAT=11                        RHO=7.02054E-02
          RXN= 2   ERG=8.1873E+00,2.0000E+01  METHOD=2
…………………………………
………………………………..
```

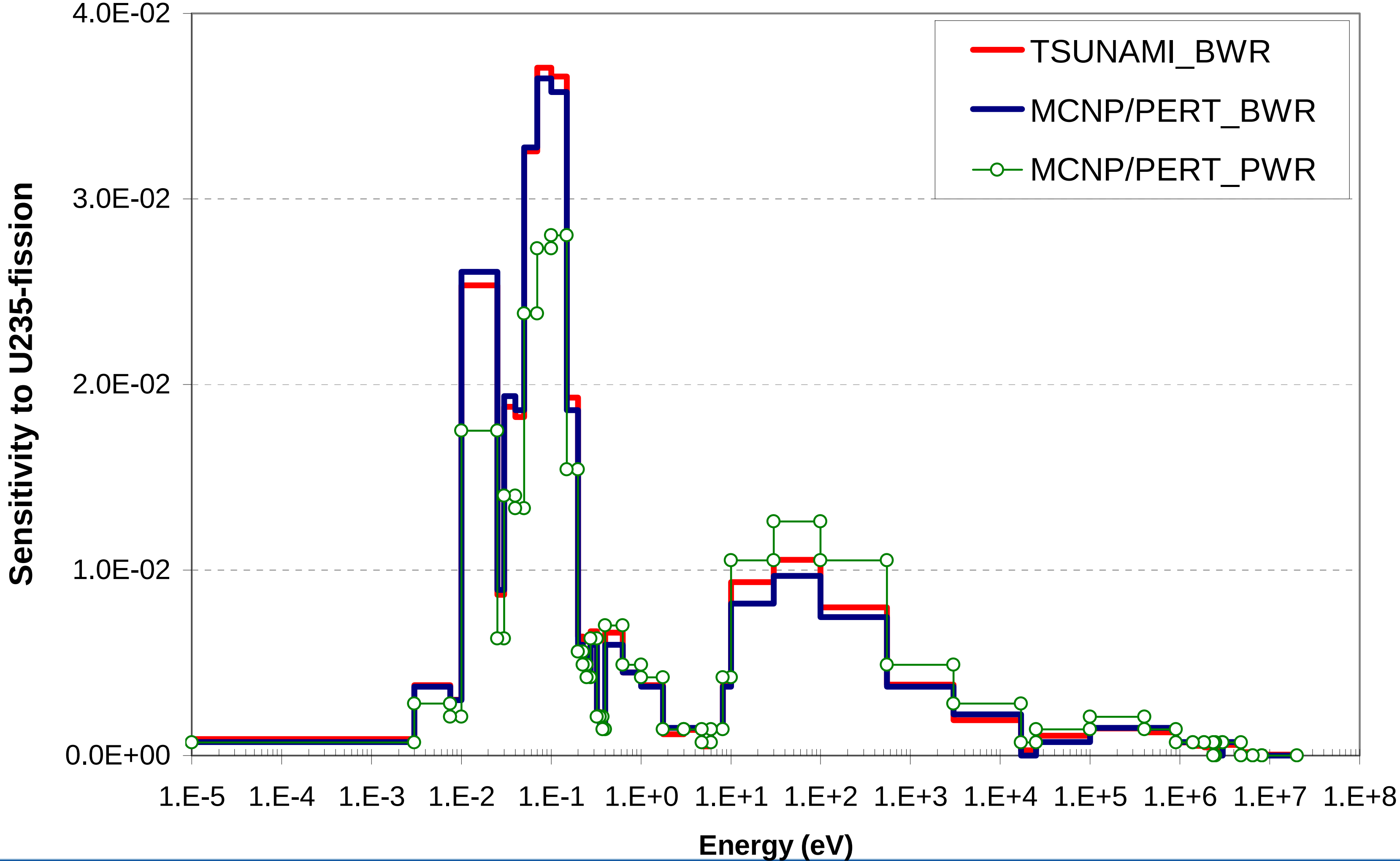
Entries must be ENDF/B reaction types that identify one or more specific reactions cross section s to perturb.

The two entries specify an energy range in wich the perturbacion is applied.

Specifies the number of terms to include in the perturbation.
In our case we include only first order (2).

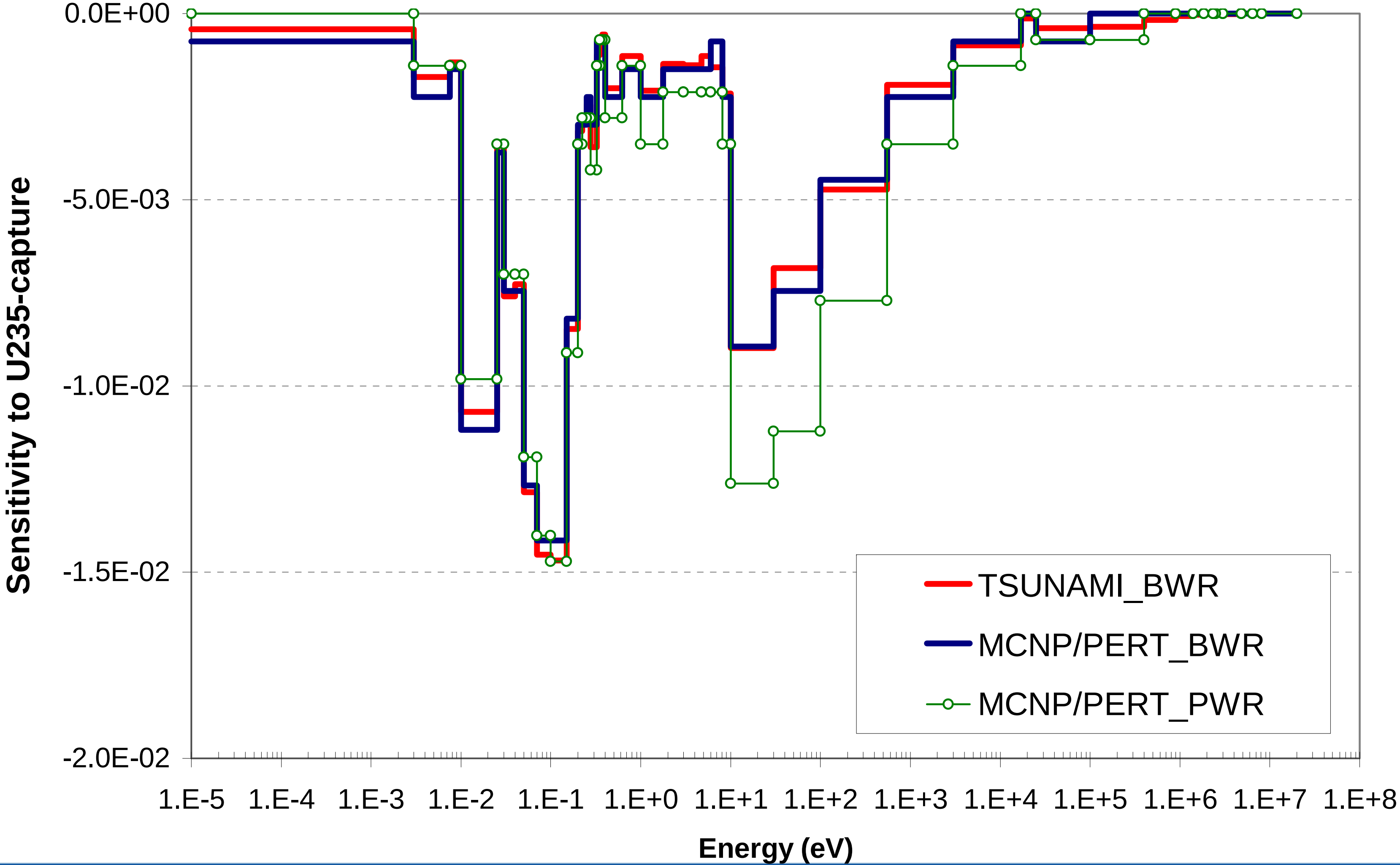
Sensitivity Coefficients (HZP)

- U235-fission: Good agreement TSUNAMI - MCNP/PERT



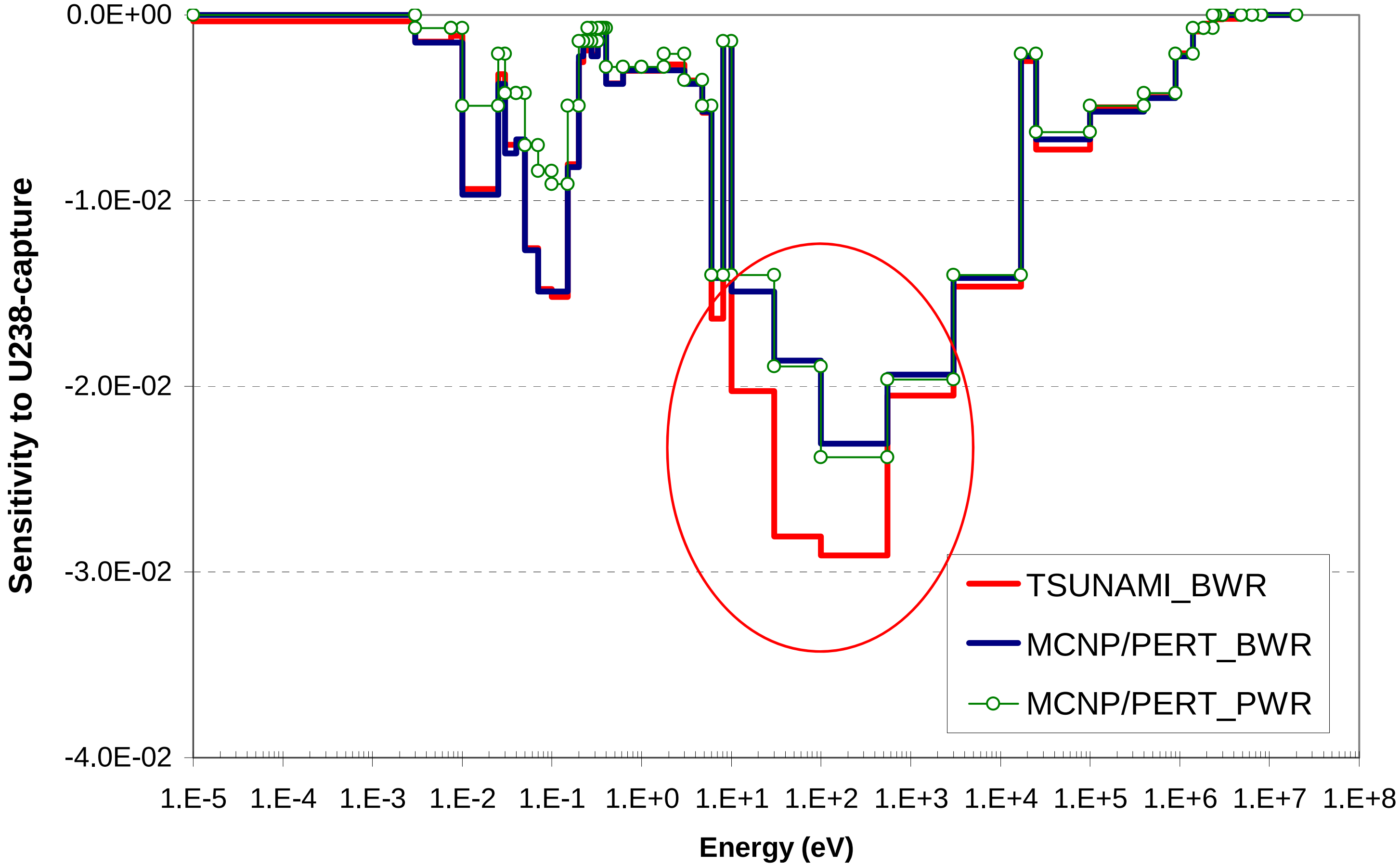
Sensitivity Coefficients (HZP/PWR)

- U235-capture: Good agreement TSUNAMI - MCNP/PERT



Sensitivity Coefficients (HZP/PWR)

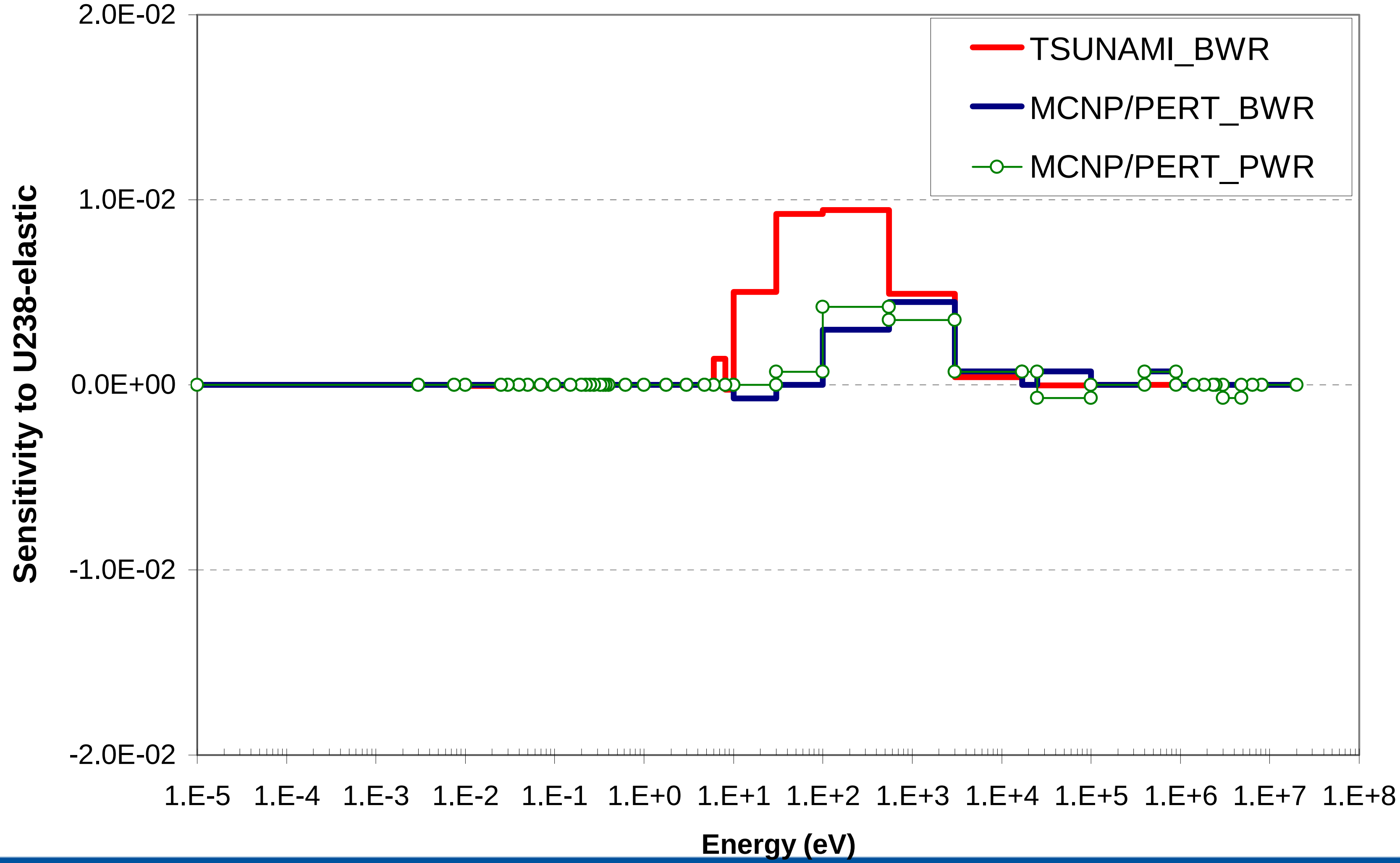
- U238-capture: Differences between 10eV-10^3 eV



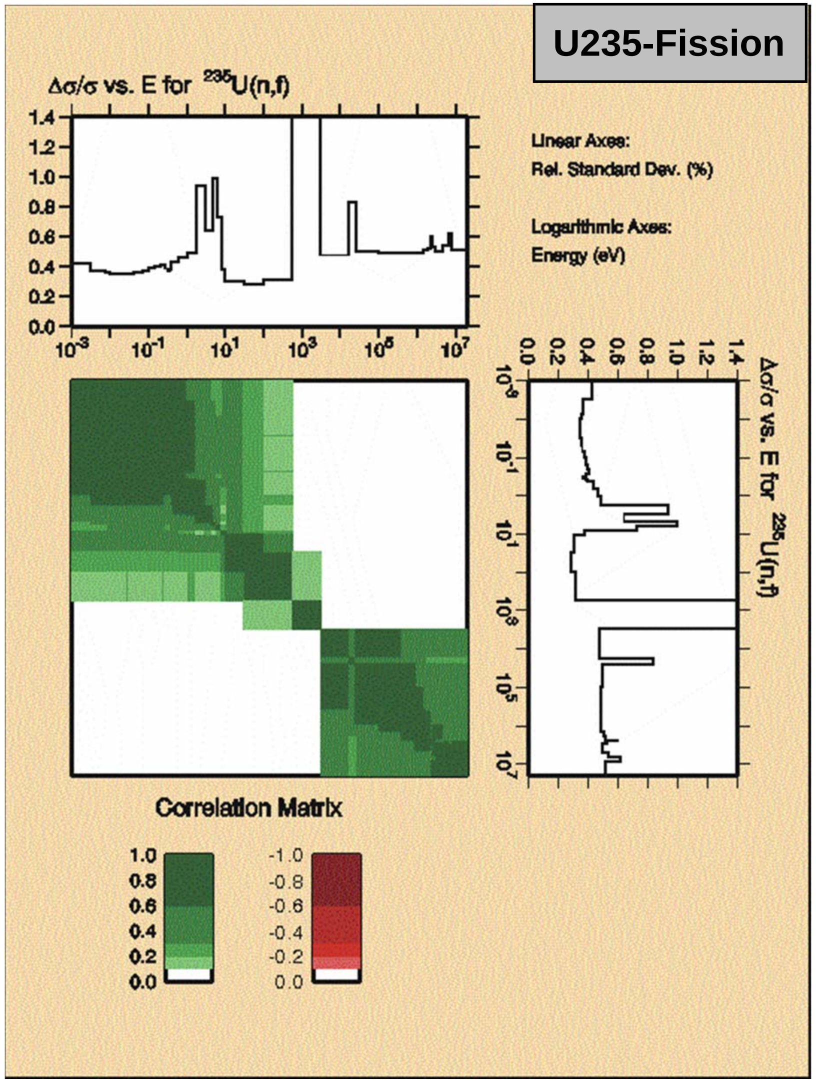
The track length estimate of keff in KCODE critically calculations assumes the fundamental eigenvector (fission distribution) is unchanged in the perturbated configuration.

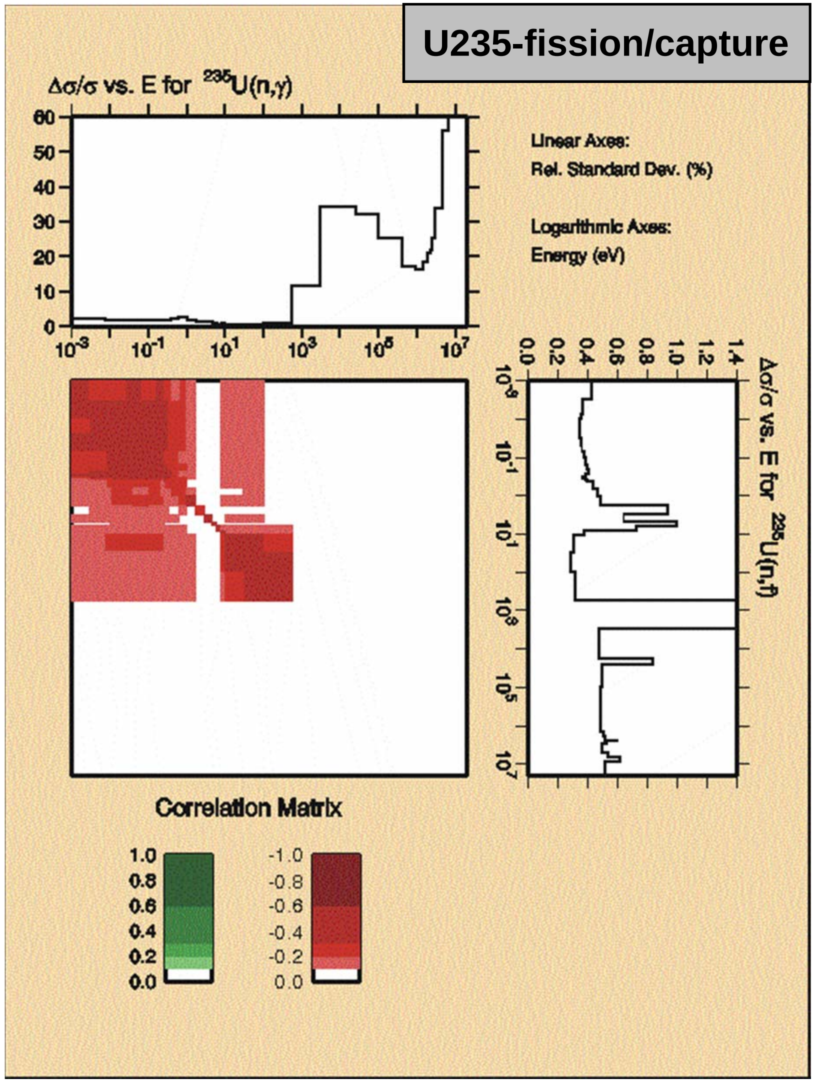
Sensitivity Coefficients (HZP/PWR)

- U238-elastic: Differences between 10eV-10^3 eV

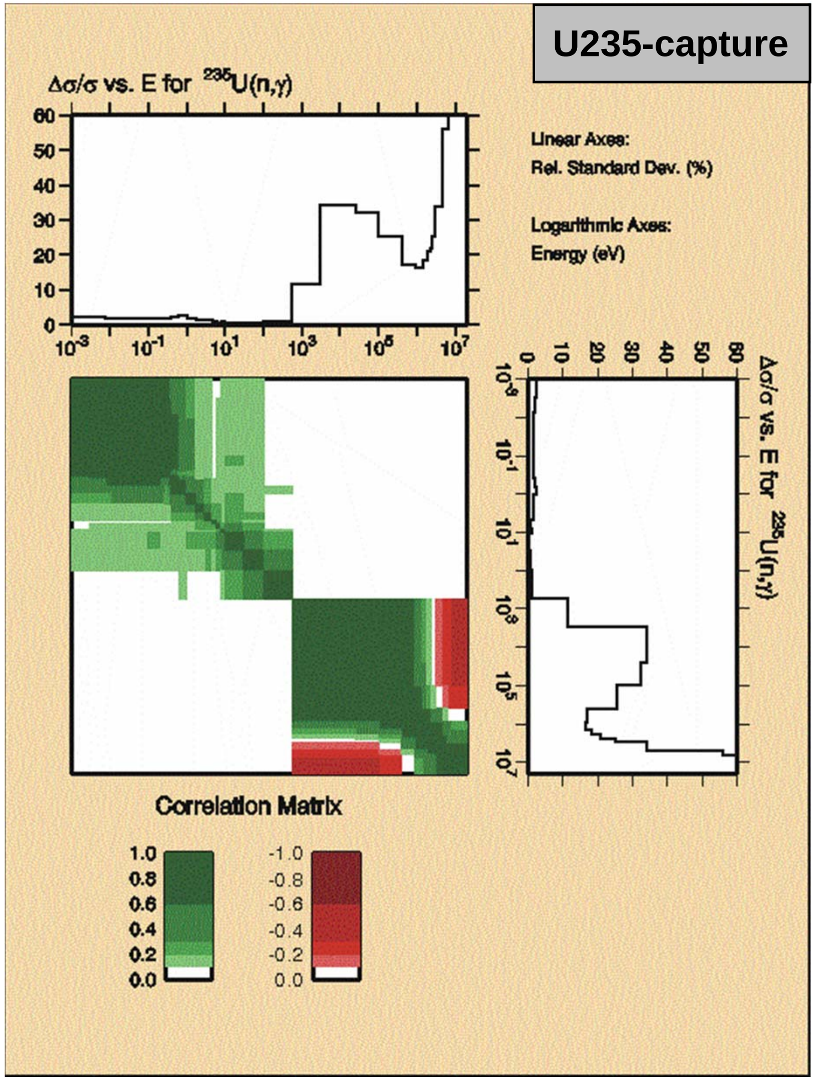


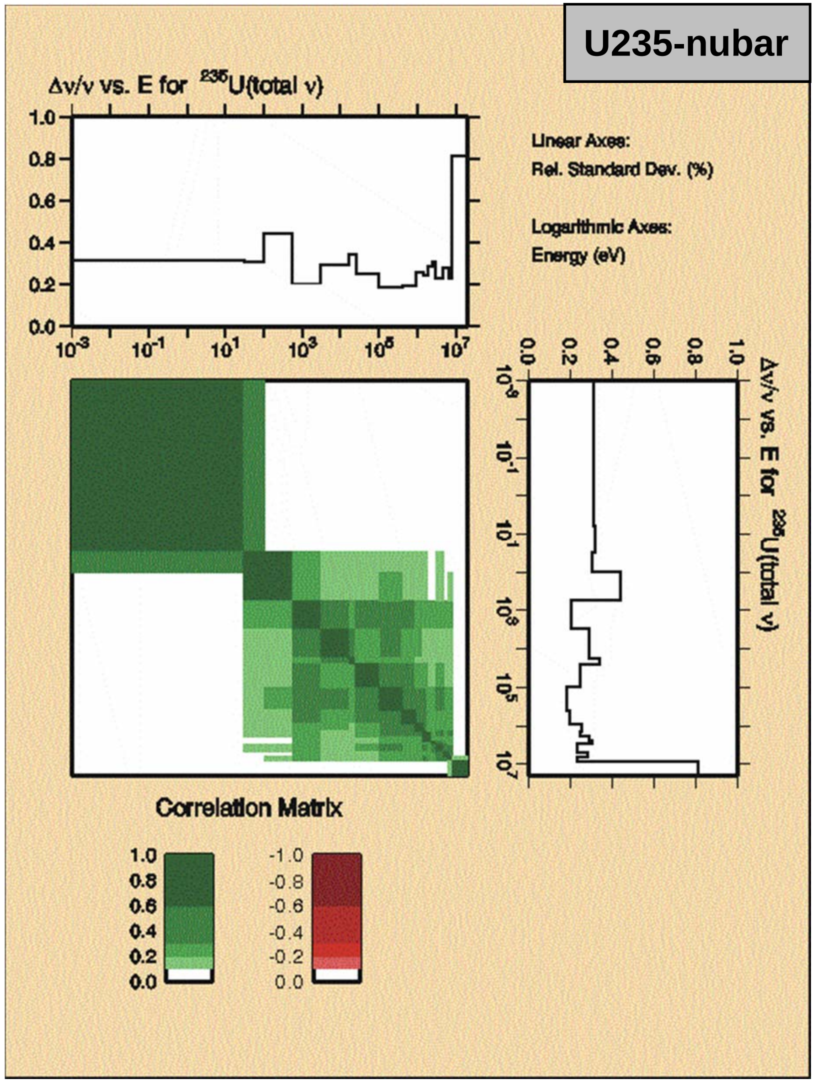
SCALE6.0 Uncertainties



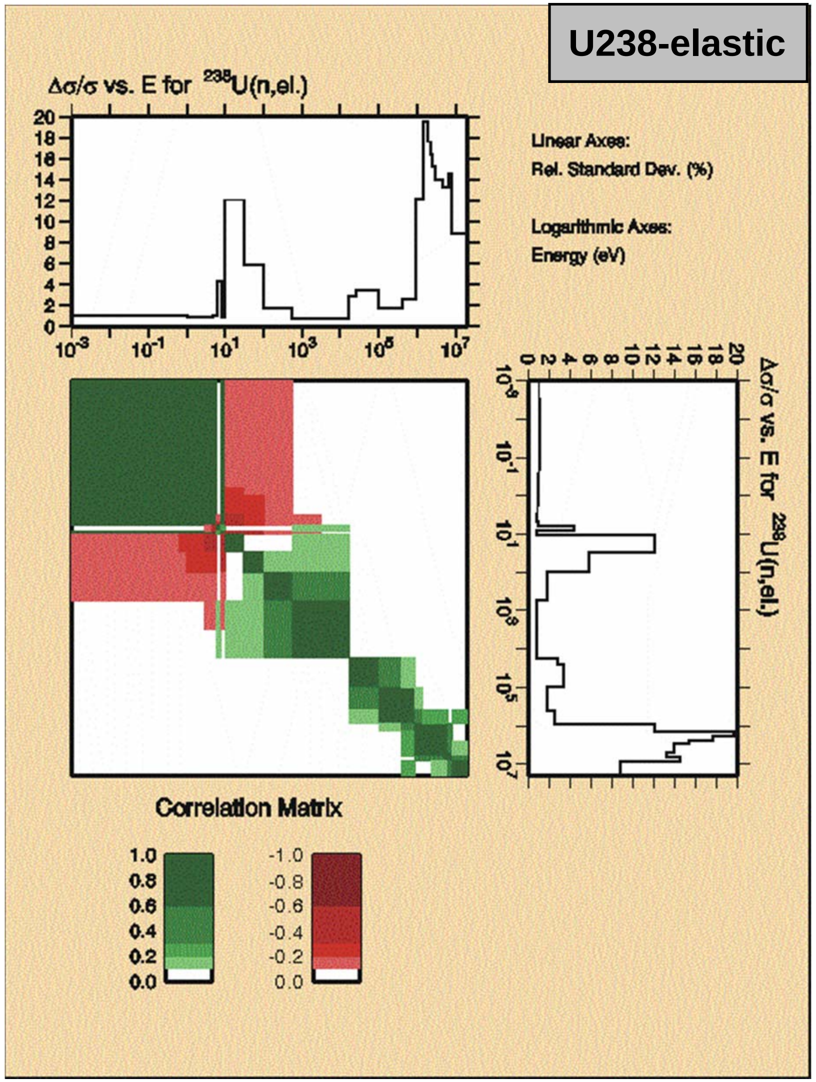


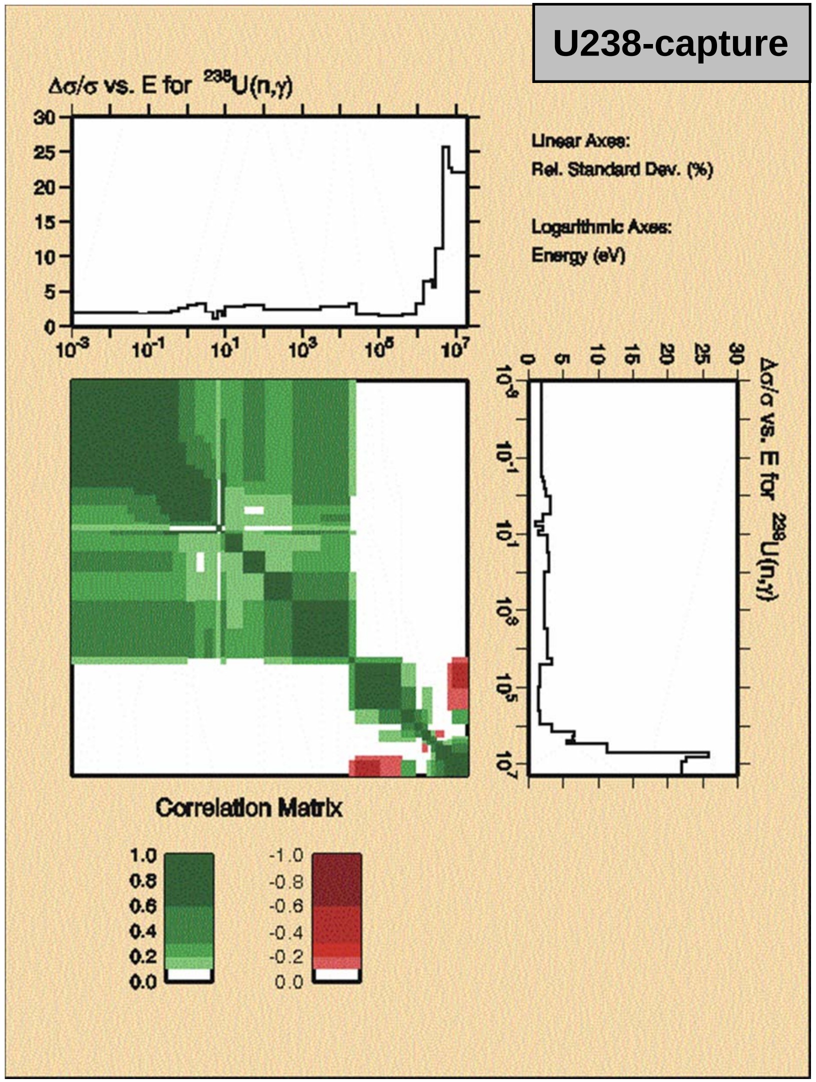
SCALE6.0 Uncertainties





SCALE6.0 Uncertainties





RESULTS: PWR

			Hot Zero Power -PWR		Hot Full Power -PWR	
			MCNP	SCALE6.0	MCNP	SCALE6.0
	Kinf		1.42701E+00 +- 0.00034	1.42190+-0.00310	1.41130E+00 +- 0.00036	1.40510+-0.00290
	Uncertanties (%Δk/k)		0.36719	0.5029	0.37336	0.5125
		U238-capt	0.2535	0.2877	0.2607	0.2977
		U235-capt	0.2095	0.2124	0.2109	0.2128
Top contributors		U235-fiss	0.0770	0.0776	0.0769	0.0777
the uncertainty		U238-n,n'	0.0944	0.1058	0.0954	0.1096
		U235-fiss-capt	0.1470	0.1050	0.1472	0.1049
		U235-nubar	-	0.2646	-	0.2633
Absortion rate ($cm^{-3}s^{-1}$)		U235	2.09330E+09	2.11E+09	2.10302E+12	2.13E+12
		U238	3.99122E+09	4.04E+09	4.1816E+12	4.24E+12
Uncertainties		U235	0.3632	-	0.3699	-
		U238	0.5431	-	0.5621	-
Fission rate ($cm^{-3}s^{-1}$)		U235	8.92751E+09	8.92E+09	8.91203E+12	8.91E+12
		U238	4.88051E+08	4.91E+08	4.99342E+11	5.04E+11
Uncertainties		U235	0.3991	-	0.4078	-
		U238	3.5985	-	3.6499	-

MCNP5 doesn’t allow to calculate chi and nu-bar!!

4. Burnup Uncertainty Analysis

Accurate control over **the spent nuclear fuel content** is essential for its safe and optimized transportation, storage and management. Consequently, the reactivity of spent fuel and its isotopic content must be accurately determined.

Nowadays, isotopic evolution throughout irradiation and decay periods can be predicted using **powerful codes and methodologies**.

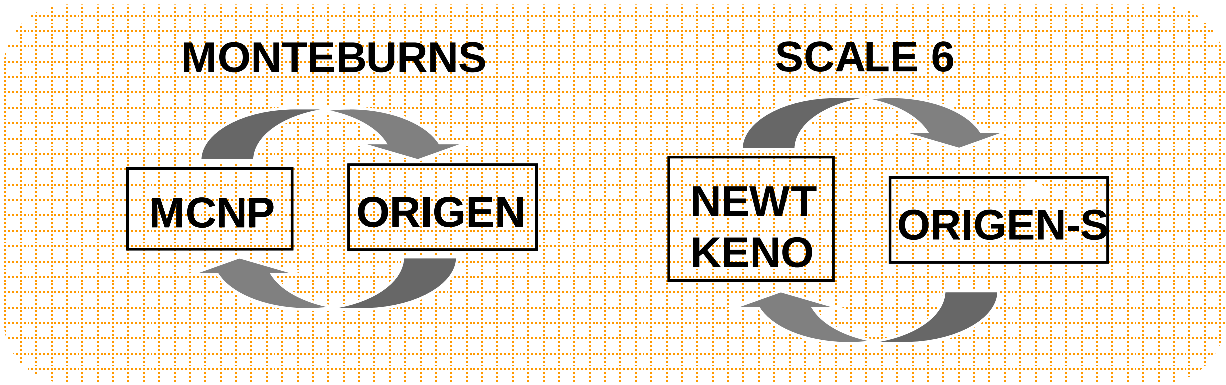


Figure 1.

Computing systems coupling neutron transport and isotopic inventory codes

Objective: Burnup Uncert.- PWR Pin-cell

In order to have a realistic confidence level in the prediction of spent fuel isotopic content, it is desirable to determine **how uncertainties affect isotopic prediction calculations** by quantifying their associated uncertainties:

- ✓ *irradiation history, calculation models-coupling, …*
- ✓ ***nuclear data: cross section, fission yields and decay data***

PWR Pin-cell:

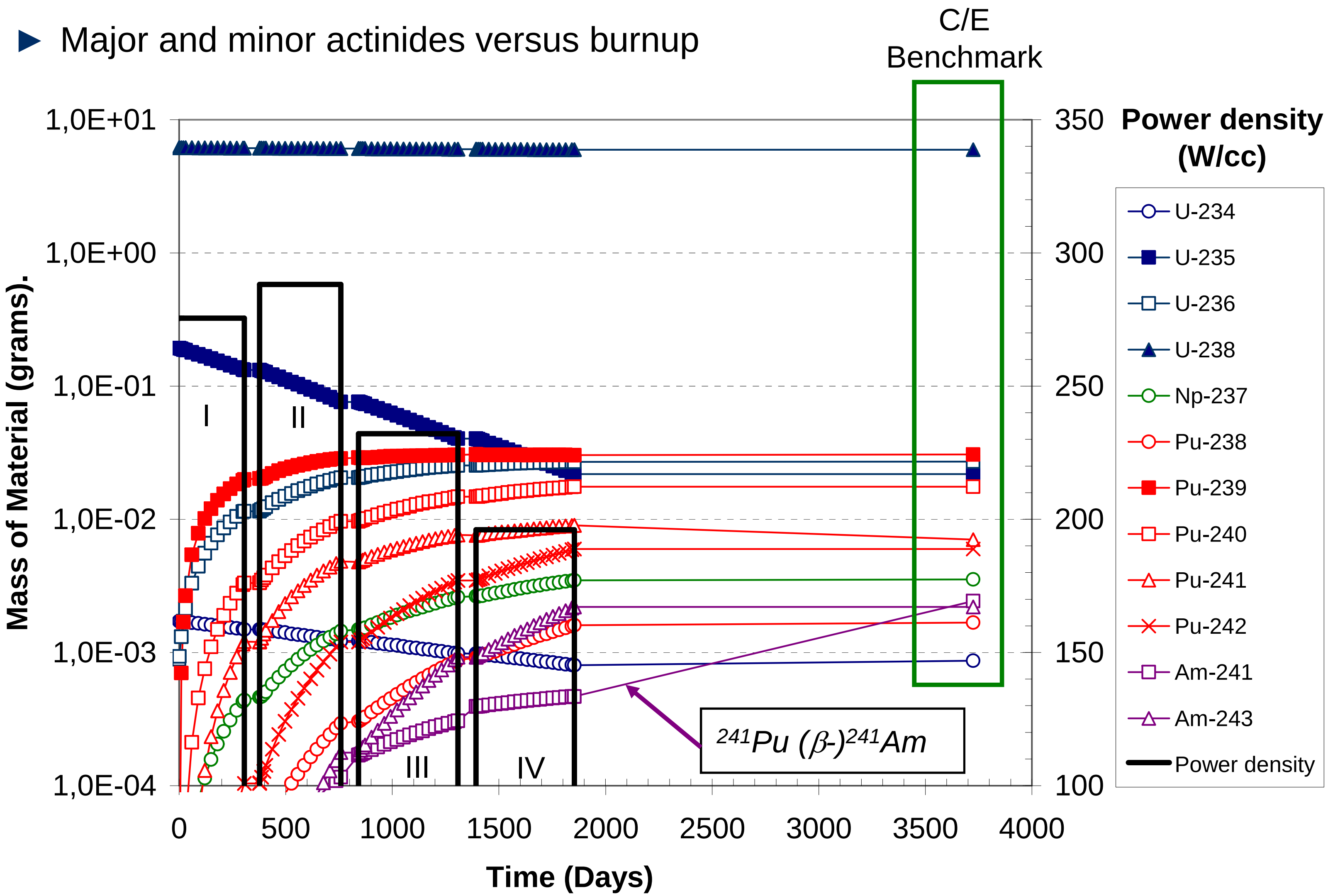
The Phase I-B (see Ref.) was proposed to provide a comparison of the ability of different code systems and data libraries to predict isotopic concentrations.

The participating organizations analyzed with their different codes and methodologies the same **LWR pin-cell problem** for three increasing burnups (CASE A - 27 GWd/TMU, CASE B - 37 GWd/TMU and **CASE C - 44 GWd/TMU**).

Ref. Phase I-B: DeHart M.D., Brady M.C., Parks C.V., OECD/NEA Burnup Credit Calculational Criticality Benchmark Phase I-B Results, ORNL-6901, Oak Ridge National Laboratory, June 1996

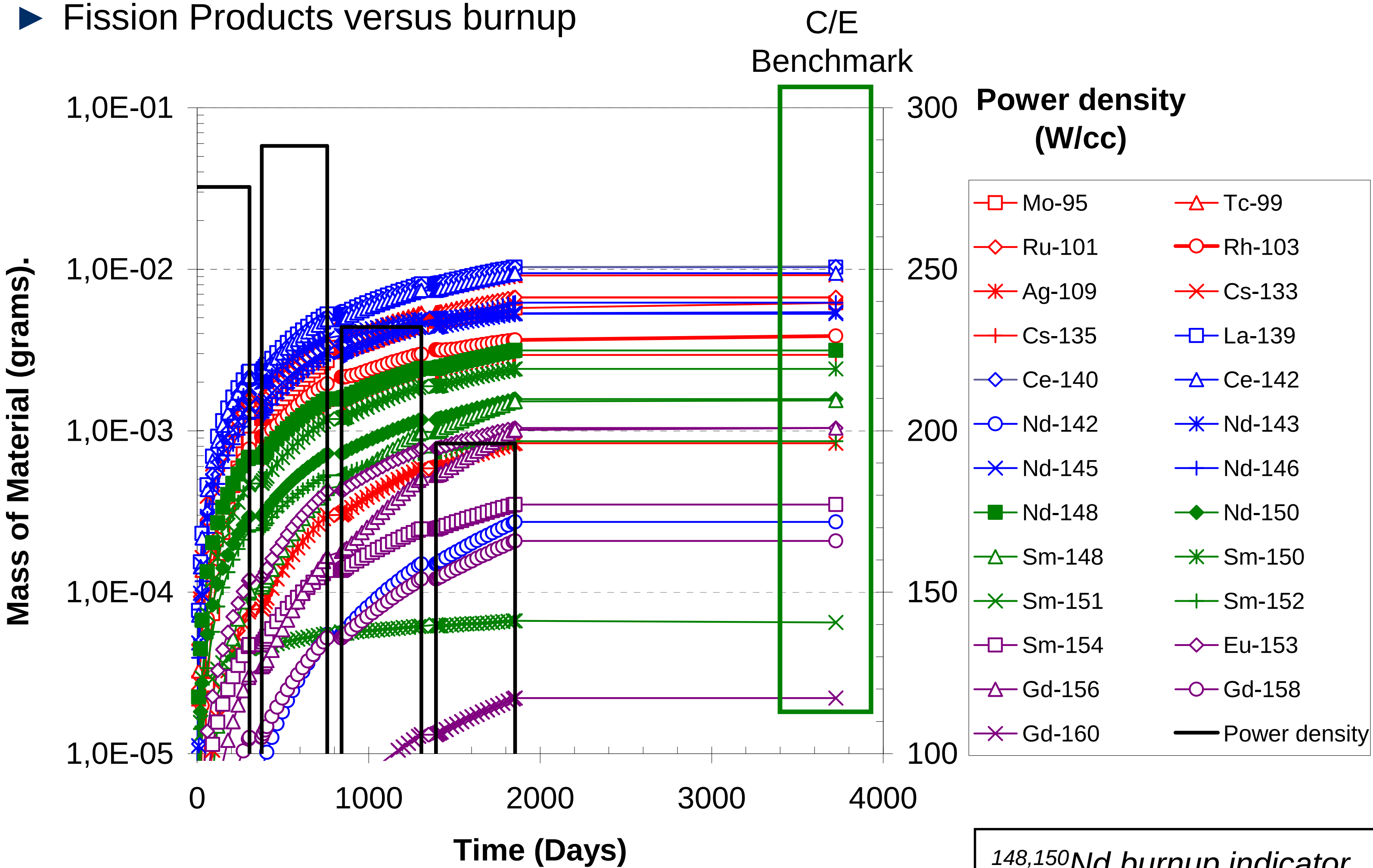
CASE C- 44 GWd/TMU: Actinides

- Major and minor actinides versus burnup



CASE C- 44 GWd/TMU: Fission Products

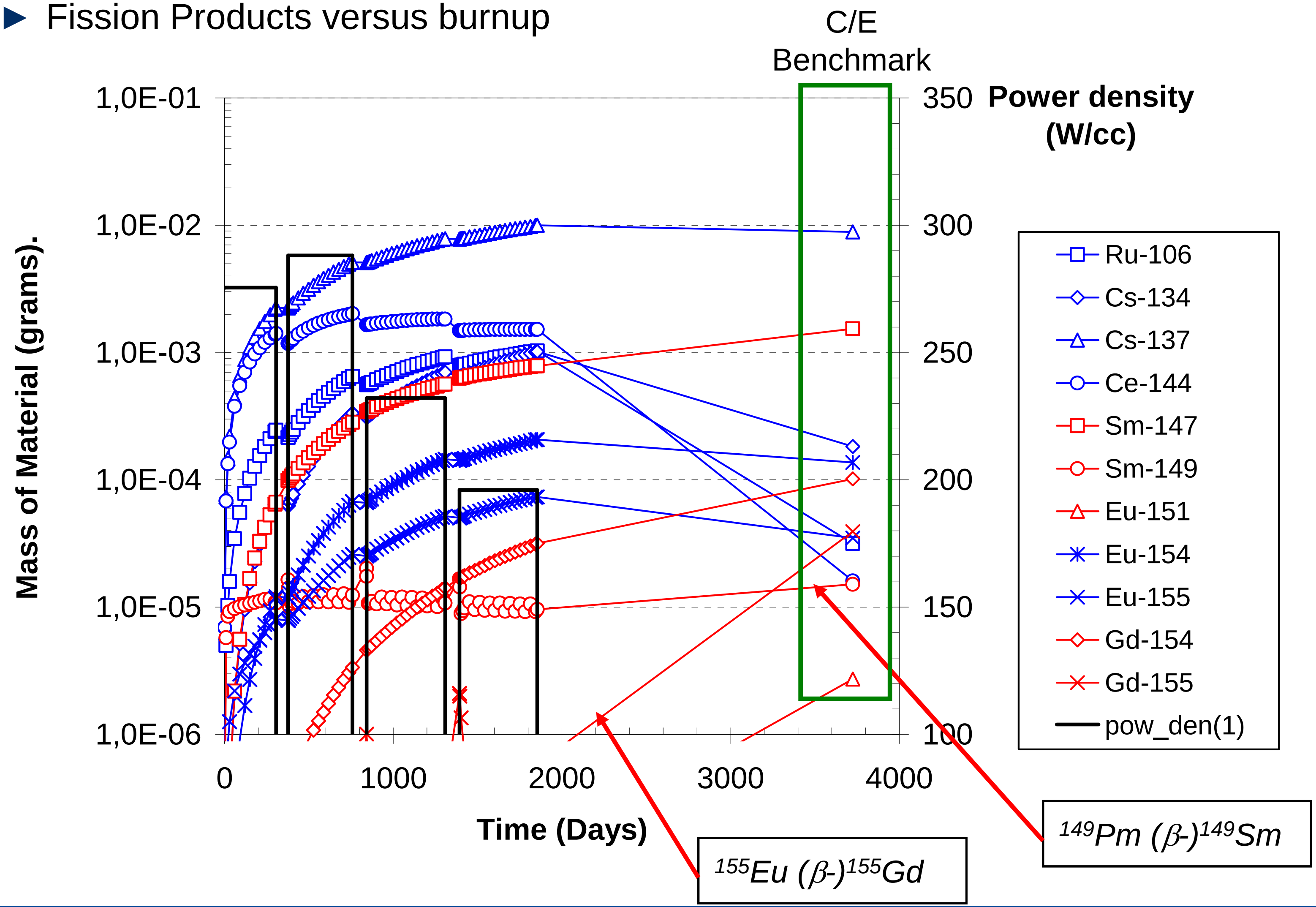
- Fission Products versus burnup



148,150Nd burnup indicator

CASE C- 44 GWd/TMU: Fission Products

- Fission Products versus burnup



5. Sources of uncertainties in a depletion calculation

The influence of all these sources should be investigated in order to understand and quantify the uncertainties associated with computer code predictions for spent fuel isotopics:

$$\frac{dN}{dt} = [\lambda]N + \left[\sigma^{eff}\right]\cdot \Phi N + \left[(\gamma\sigma_{fiss})^{eff}\right]\cdot \Phi N = A\cdot N$$

$$N = N\left(\lambda, \sigma^{eff}, \Phi\right) = N(\lambda, \gamma, \sigma^{g}, \phi^{g}(E), \Phi)$$

- Uncertainties in decay constants: Δ_{λ}
- Uncertainties in one-group effective xs: $\Delta_{\sigma^{eff}}$

$$\sigma^{eff} = \sum_{g} \sigma^{g}\phi^{g} \Big/ \sum_{g} \phi^{g}$$

- uncertainties in the evaluated nuclear xs data: $\Delta\sigma^{g}$

- uncertainties in the flux spectrum obtained from the transport calculation: $\Delta\phi^{g}$

- Uncertainties in the integrated neutron flux: $\Delta\Phi$

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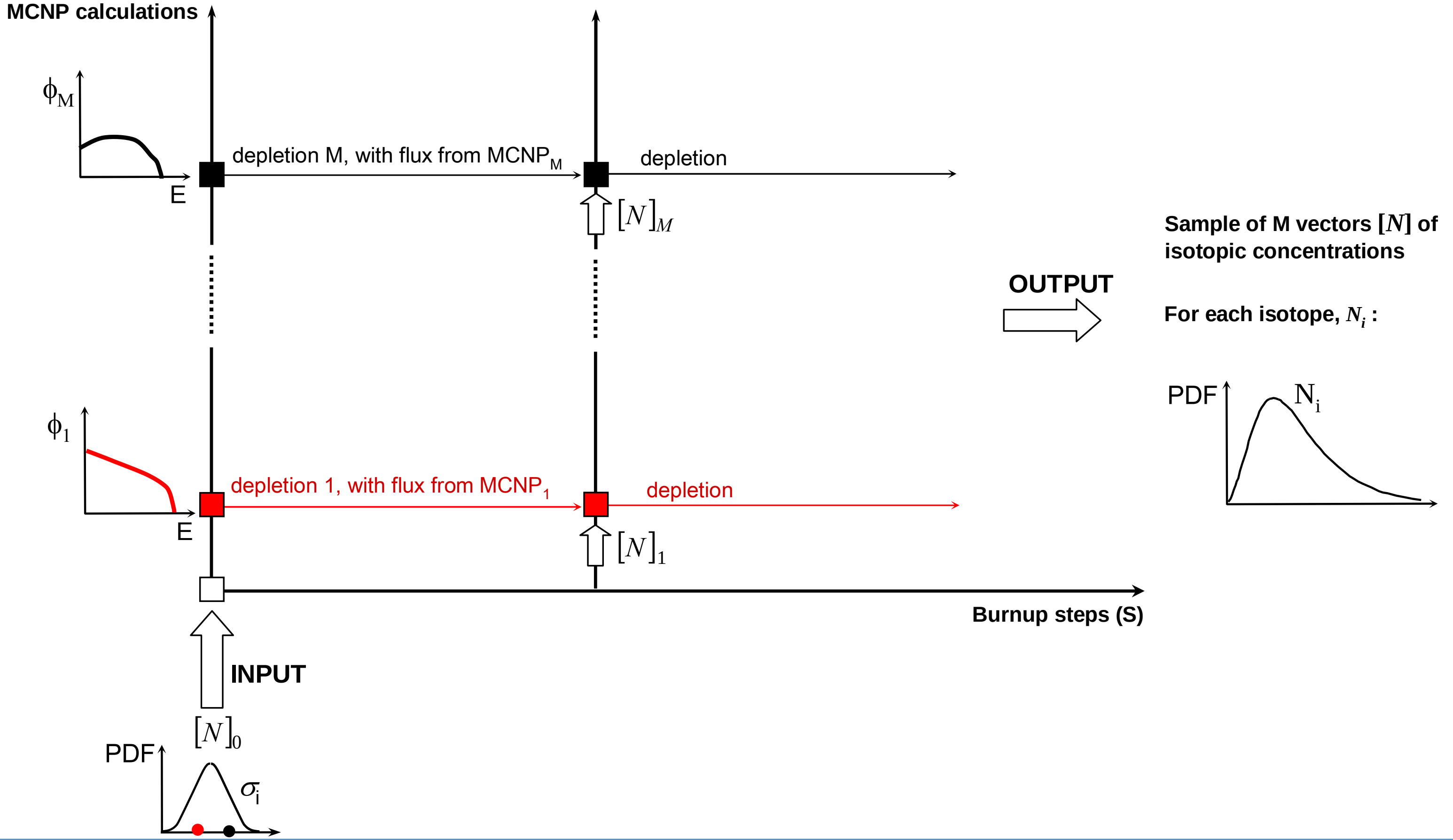
5.1 Propagation of uncertainties in burn-up calculations: "Brute Force MC"

"Brute force" random sampling method

Same sequence that the coupled calculation scheme to infer an error propagation procedure throughout the time

Simultaneous random sampling of the PDF of all the input parameters



5.2 Propagation of uncertainties in burn-up calculations: "S/U Analysis"

Sensitivity/ Uncertainty Analysis (S/U)

Procedure based on a **first order Taylor** series approach

$$N_i(\sigma^{eff}) = N_i(\hat{\sigma}^{eff}) + \sum_{j=1}^{R} \left[\frac{\partial N_i}{\partial \sigma_j}\right]_{\hat{\sigma}^{eff}} \left(\sigma_j^{eff} - \hat{\sigma}_j^{eff}\right) + \ldots$$

Sensitivity coefficient ρ_{ij}

ε_j error in the 1-G effective xs

$$\sigma_j^{eff} = \sum_g \sigma_j^g \phi^g$$

$$\varepsilon_j = \sum_{g=1}^{G} \phi^g \left(\sigma_j^g - \hat{\sigma}_j^g\right) + \sum_{g=1}^{G} \sigma_j^g \left(\phi^g - \hat{\phi}^g\right) = \phi^T \boxed{\varepsilon_{\sigma_j}} + \sigma_j^T \boxed{\varepsilon_\phi}$$

errors due to uncertainties in the multigroup xs $\lfloor COV_{\sigma_j} \rfloor$

to be processed from the uncertainty libraries

errors due to uncertainties in the multigroup flux spectrum $\lfloor COV_{\phi} \rfloor$

to be obtained from a single MCNP calculation

5.2 Propagation of uncertainties in burn-up calculations : “S/U Analysis”

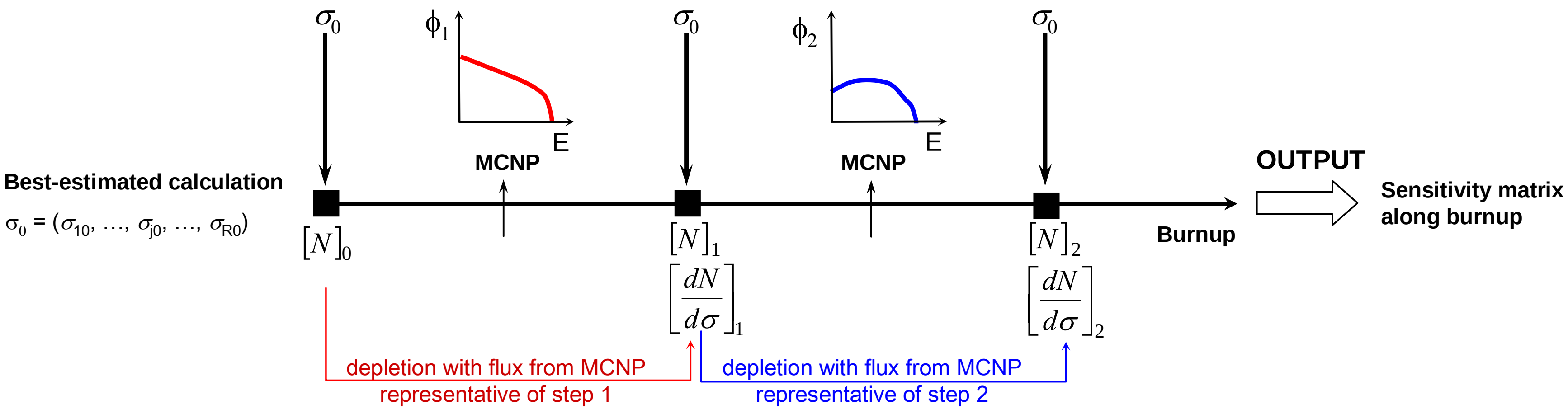
Sensitivity/ Uncertainty Analysis (S/U)

$$N\left(\sigma^{eff}\right) - N\left(\hat{\sigma}^{eff}\right) \approx \boldsymbol{S}\,\varepsilon$$

$$var\ N \approx \boldsymbol{S}\left[COV_{\sigma^{eff}}\right]\boldsymbol{S}^{\boldsymbol{T}} \approx \boldsymbol{S}\left\{ \underbrace{\begin{bmatrix} \ddots & & 0 & \\ 0 & \hat{\phi}^{T}\left[COV_{\sigma_j}\right]\hat{\phi} & & \\ & & & \ddots \end{bmatrix}} + \underbrace{\begin{bmatrix} \ddots & & 0 & \\ 0 & \hat{\sigma}_j^{\,T}\left[COV_{\phi}\right]\hat{\sigma}_j & & \\ & & & \ddots \end{bmatrix}} \right\} \boldsymbol{S}^{\boldsymbol{T}}$$

Propagates the multigroup xs uncertainties when there is no statistical flux errors

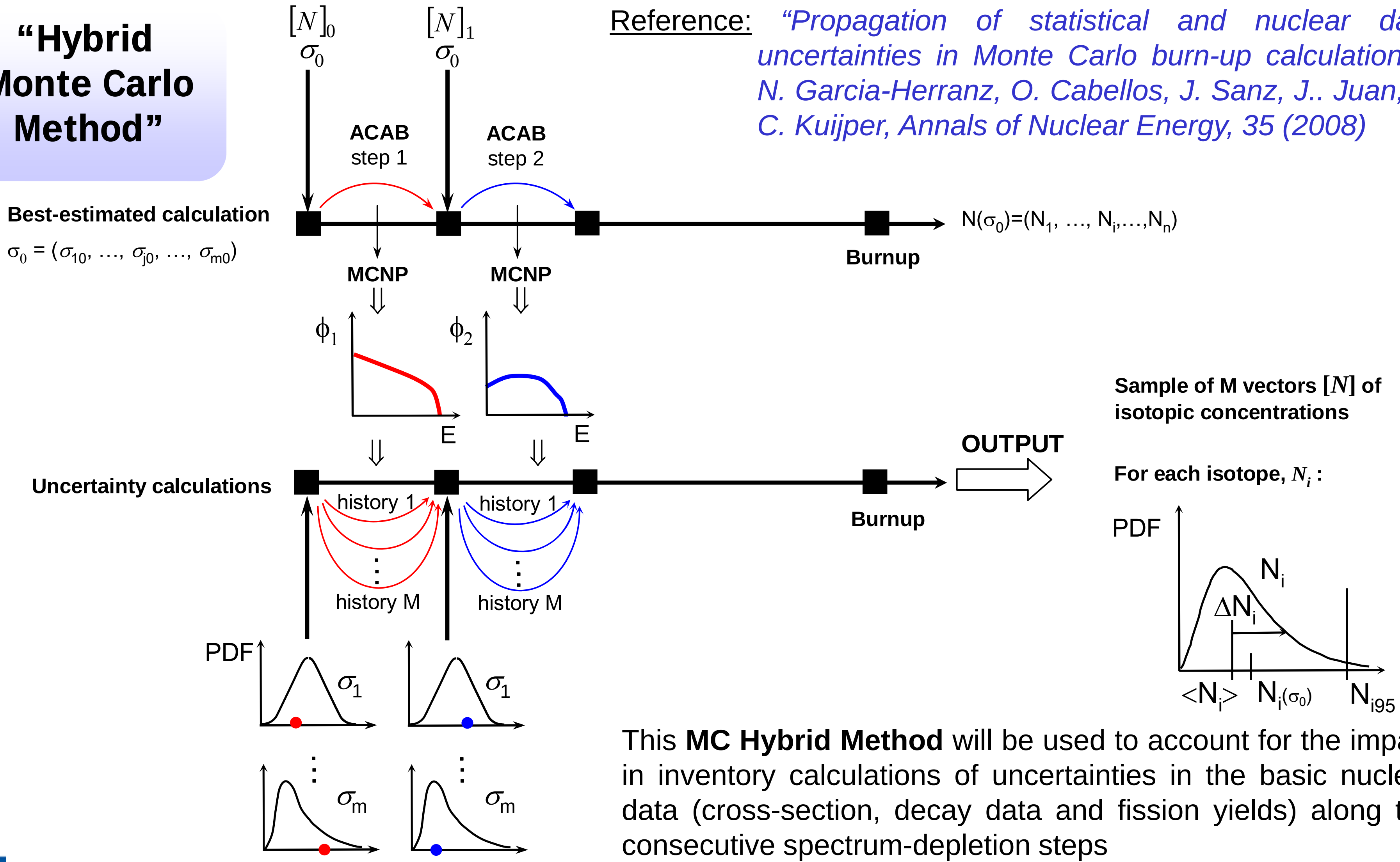
Propagates statistical flux errors when there is no multigroup xs covariances



5.3 Propagation of uncertainties in burn-up calculations: “Hybrid Method”

“Hybrid Monte Carlo Method”

Reference: *“Propagation of statistical and nuclear data uncertainties in Monte Carlo burn-up calculations”, N. Garcia-Herranz, O. Cabellos, J. Sanz, J.. Juan, J. C. Kuijper, Annals of Nuclear Energy, 35 (2008)*



This **MC Hybrid Method** will be used to account for the impact in inventory calculations of uncertainties in the basic nuclear data (cross-section, decay data and fission yields) along the consecutive spectrum-depletion steps

6. Propagation of uncertainties in burn-up calculations: "Phase I-B Benchmark"

Table. MCNP-ACAB **calculated uncertainties in actinides** due to cross-section & decay data uncertainties for Phase-1B OECD/NEA Burnup Credit Benchmark. (**CASE C- 44.34 GWd/TMU**)

- Uncertainties due to **cross-sections**:
  - For major actinides, the uncertainty remains below 2%. It increases for minor actinides
  - Lower uncertainties using SCALE6.0/COVA
  - Lower uncertainties for Cm isotopes using EAF2010/UN
- Uncertainties due to **decay data** remain very low, except for 243Cm with 0.8% (relative error of Cm243 half-life is 6.7%)

Isotope	Decay Data JEFF-3.1.1	Cross-section EAF2007/UN 3 groups	Cross-section EAF2010/UN 3 groups	Cross-section SCALE6.0/COVA 44 groups
233U	0.2	1.4	0.6	1.3
234U	0.1	2.5	0.8	1.8
235U	0.0	0.8	0.1	0.2
236U	0.0	0.4	0.4	0.2
238U	0.0	0.1	0.1	0.0
237Np	0.0	0.7	0.6	0.5
238Pu	0.0	0.9	2.4	0.3
239Pu	0.0	1.5	0.5	0.5
240Pu	0.0	1.8	1.1	0.5
241Pu	0.1	1.6	0.9	0.4
242Pu	0.0	1.2	1.1	0.7
241Am	0.2	1.5	0.9	0.4
243Am	0.0	1.9	1.3	1.7
242Cm	0.4	1.5	3.1	0.7
243Cm	0.8	4.6	4.4	3.2
244Cm	0.1	2.0	1.4	1.8
245Cm	0.0	3.1	1.6	3.8
246Cm	0.0	4.0	1.8	2.7
247Cm	0.0	4.5	2.1	3.2
248Cm	0.0	5.8	2.9	3.7
250Cf	0.2	7.5	4.6	4.7
251Cf	0.1	7.9	5.0	5.2
252Cf	0.4	6.7	4.6	4.4

(in grey color) Phase I-B selected actinides

6. Propagation of uncertainties in burn-up calculations: "Phase I-B Benchmark"

Table. MCNP-ACAB calculated uncertainties in light elements due to cross-section uncertainties for Phase-1B OECD/NEA Burnup Credit Benchmark. (CASE C- 44.34 GWd/TMU)

Isotope	Fission Yields JEFF-3.1.1	Decay Data JEFF-3.1.1	Cross-section EAF2007/UN 3 groups	EAF2010/UN 3 groups	SCALE6.0/COVA 44 groups
95Mo	4,5	0,0	0,5	0,4	0,2
99Tc	1,2	0,0	0,4	0,4	0,2
101Ru	1,2	0,0	0,4	0,3	0,2
106Ru	1,8	0,9	0,5	0,5	0,2
103Rh	1,3	0,0	1,9	0,7	0,3
109Ag	1,3	0,0	2,3	2,3	0,3
133Cs	0,9	0,0	0,4	0,3	0,2
134Cs	0,9	0,0	1,7	1,1	0,8
135Cs	0,9	0,0	1,1	0,7	0,4
137Cs	1,2	0,0	0,4	0,3	0,2
139La	1,2	0,0	0,4	0,3	0,1
140Ce	1,2	0,0	0,3	0,3	0,1
142Ce	1,3	0,0	0,4	0,3	0,1
144Ce	1,7	0,4	0,5	0,5	0,2
142Nd	1,3	0,0	0,8	1,6	0,5
143Nd	1,1	0,0	0,5	0,9	0,3
145Nd	1,1	0,0	0,4	0,3	0,2
146Nd	0,8	0,0	0,4	0,3	0,2
148Nd	0,9	0,0	0,4	0,3	0,2
150Nd	1,4	0,0	0,4	0,3	0,2

(in grey color) Phase I-B selected actinides

- **Uncertainties due to decay data** remain very low, except for **151Eu - <u>7.1% rel. err.</u>** (it is generated by β-decay of Sm151 with a half-life relative error of 6.7%)

- **Uncertainties due to fission yields** remain below 5%: 95Mo with 4.5% (high sensitivity to 95Zr FY) and 149Sm with 4.7% (high sensitivity to 149Pm FY)

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6. Propagation of uncertainties in burn-up calculations: "Phase I-B Benchmark"

Table. MCNP-ACAB calculated uncertainties in light elements due to cross-section uncertainties for Phase-1B OECD/NEA Burnup Credit Benchmark. (**CASE C- 44.34 GWd/TMU**)

Isotope	Fission Yields JEFF-3.1.1	Decay Data JEFF-3.1.1	Cross-section EAF2007/UN 3 groups	Cross-section EAF2010/UN 3 groups	Cross-section SCALE6.0/COVA 44 groups
147Sm	1,2	0,0	1,0	0,4	1,0
148Sm	1,3	0,0	0,7	0,4	0,4
149Sm	4,7	0,0	11,2	2,5	4,5
150Sm	0,8	0,0	0,8	0,4	0,7
151Sm	2,7	0,3	2,2	2,4	2,1
152Sm	0,8	0,0	1,6	0,6	0,7
154Sm	1,0	0,0	0,4	0,4	0,2
151Eu	2,7	7,1	2,2	2,3	2,1
153Eu	0,7	0,0	4,6	3,2	0,5
154Eu	0,7	0,0	10,6	7,6	3,1
155Eu	1,3	0,2	17,3	7,5	4,0
154Gd	0,7	0,0	7,7	5,6	2,4
155Gd	1,3	0,2	17,3	7,5	4,0
156Gd	0,9	0,0	5,2	1,9	0,5
158Gd	1,3	0,0	10,2	1,0	0,5
160Gd	2,7	0,0	0,6	0,5	0,2

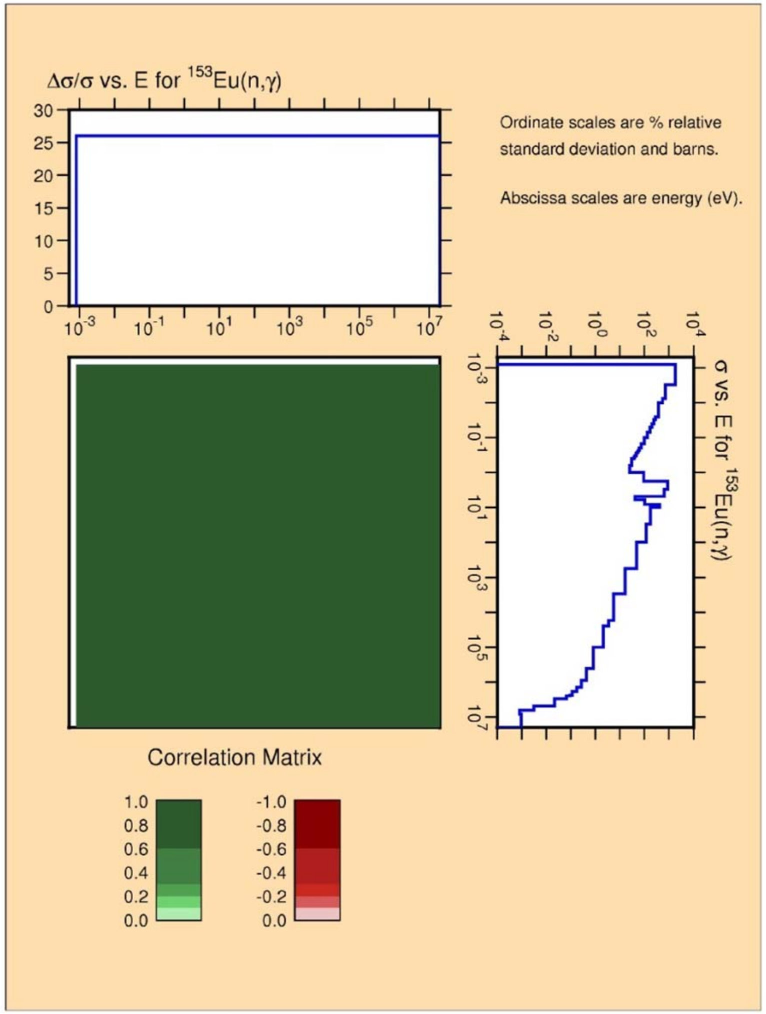
(in grey color) Phase I-B selected actinides

- **Higher uncertainties due to cross-section data** showing a good agreement between EAF2010/UN and SCALE6.0/COVA

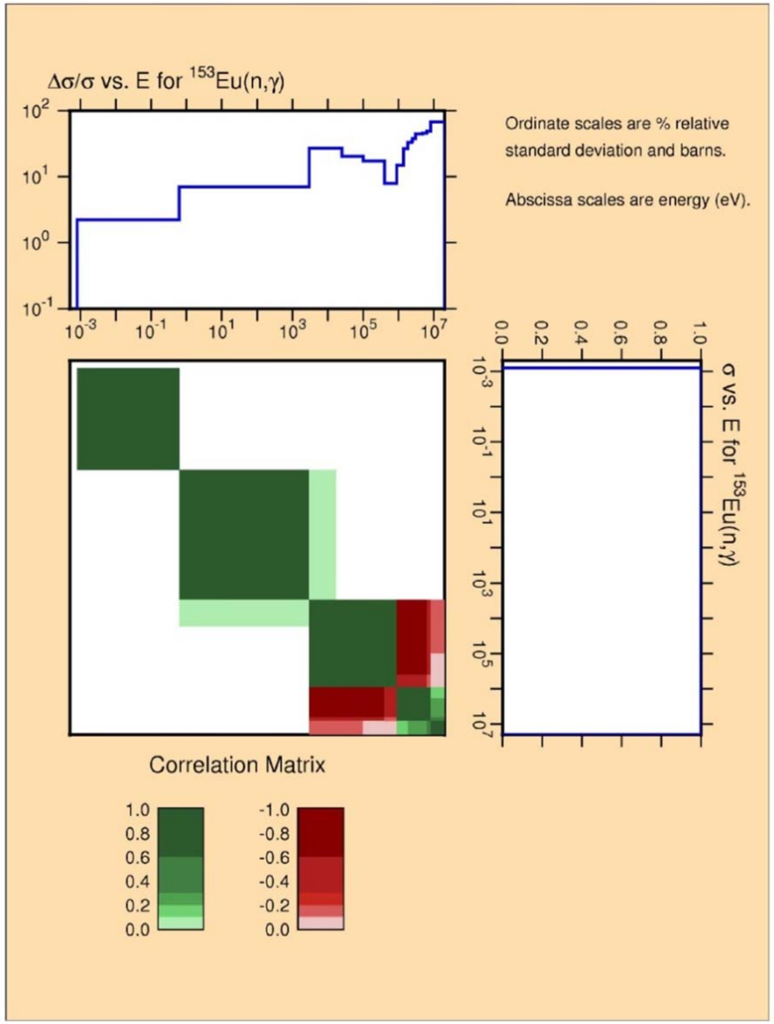
- **155Gd:** it is generated by β-decay of 155Eu, with higher sensitivities to **155Eu and 153Eu (n,γ)** reactions, and 155Eu- fission yield
- **149Sm:** important contribution by β-decay of 149Pm, with higher sensitivities to **149Sm (n,γ)** reaction and 149Pm-fission yield

Cross-section Uncertainties: e.g. 153Eu (n,γ)

EAF2010/UN

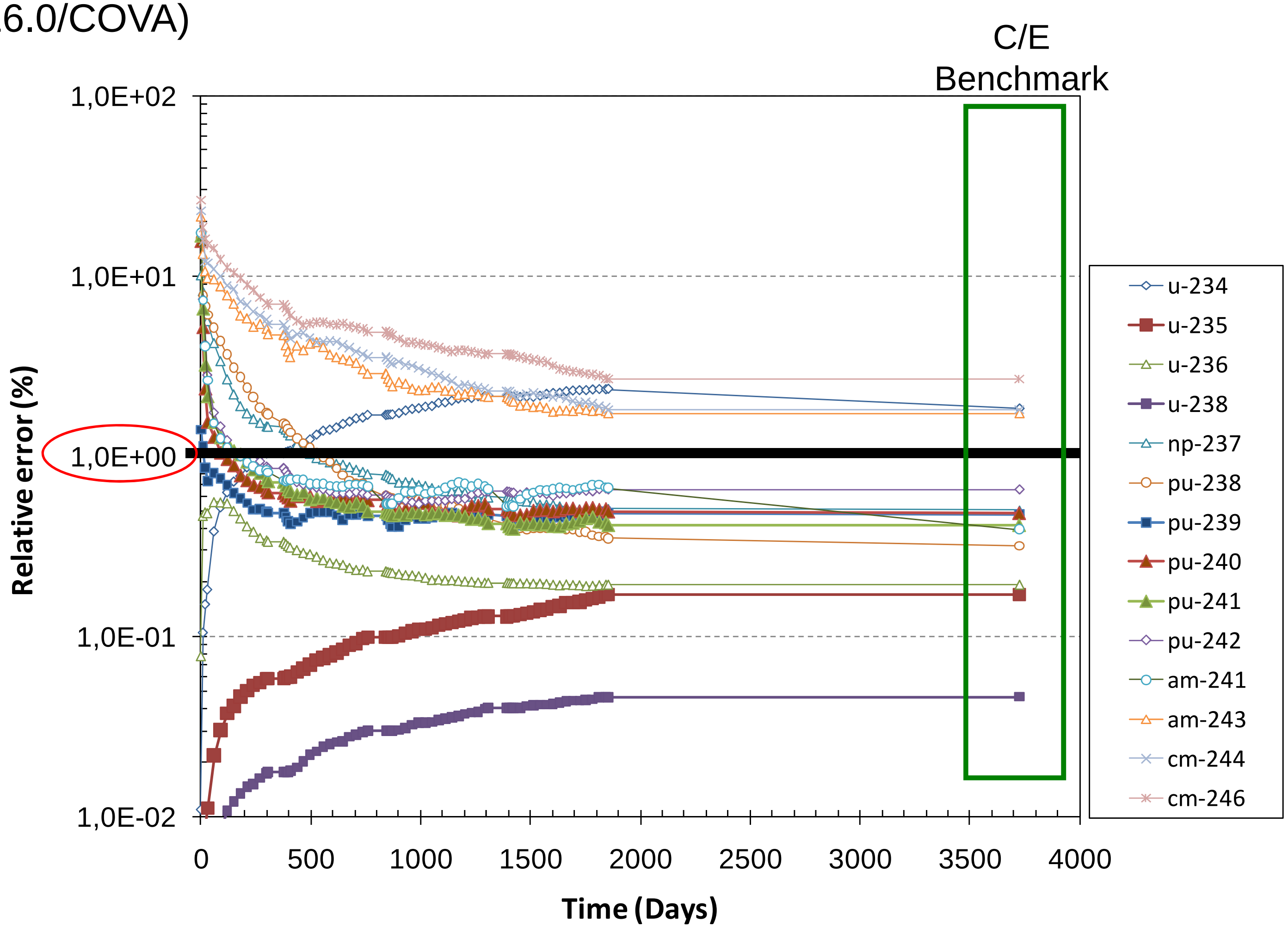


SCALE6.0/COVA



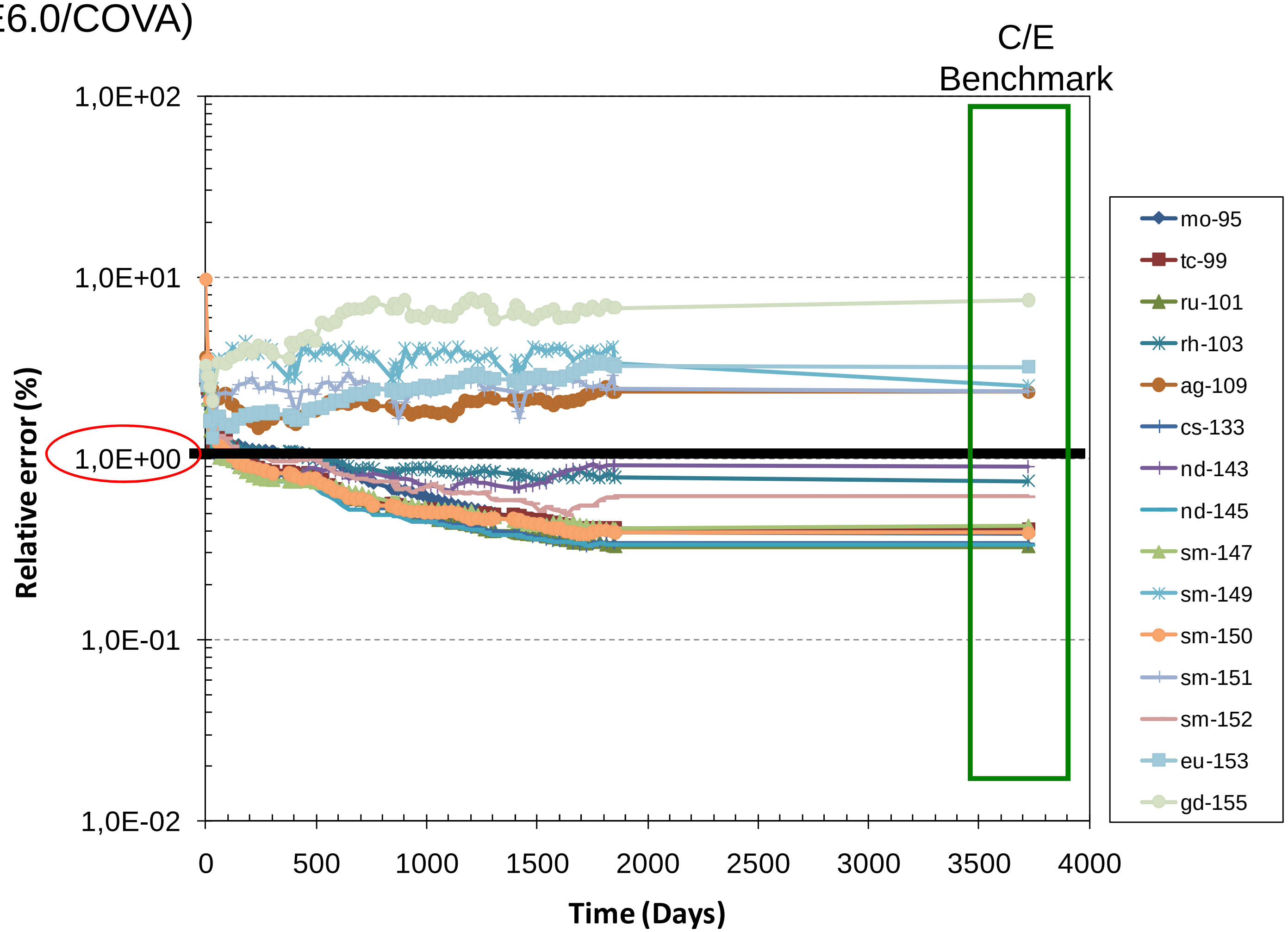
ΔN/N due to XS: Actinides

- ΔN/N (%) predicted with Hybrid Monte Carlo Method due to **uncertainties in XSs** (SCALE6.0/COVA)



ΔN/N due to XS: Fission Products

- ΔN/N (%) predicted with Hybrid Monte Carlo Method due to **uncertainties in XSs** (SCALE6.0/COVA)



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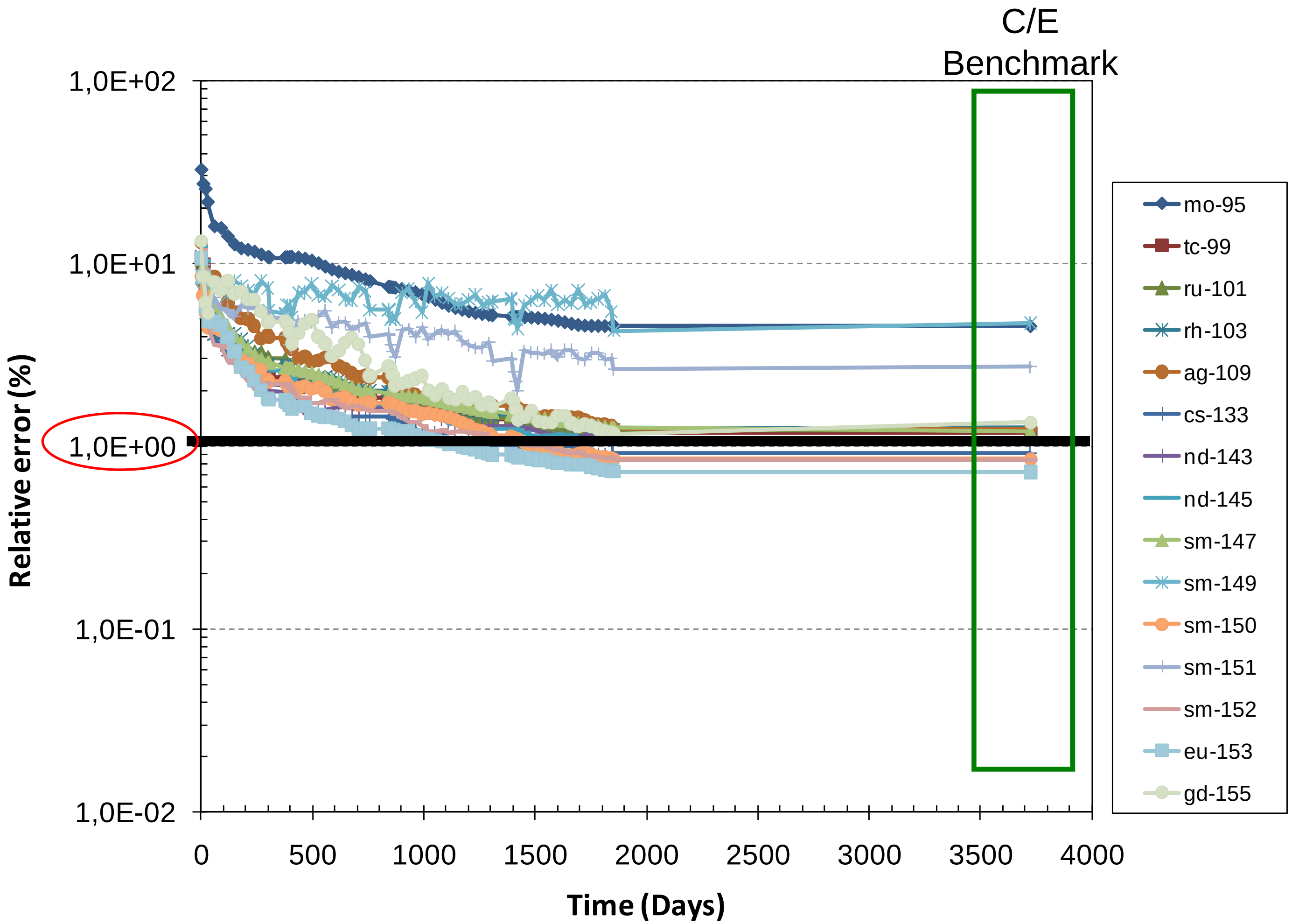
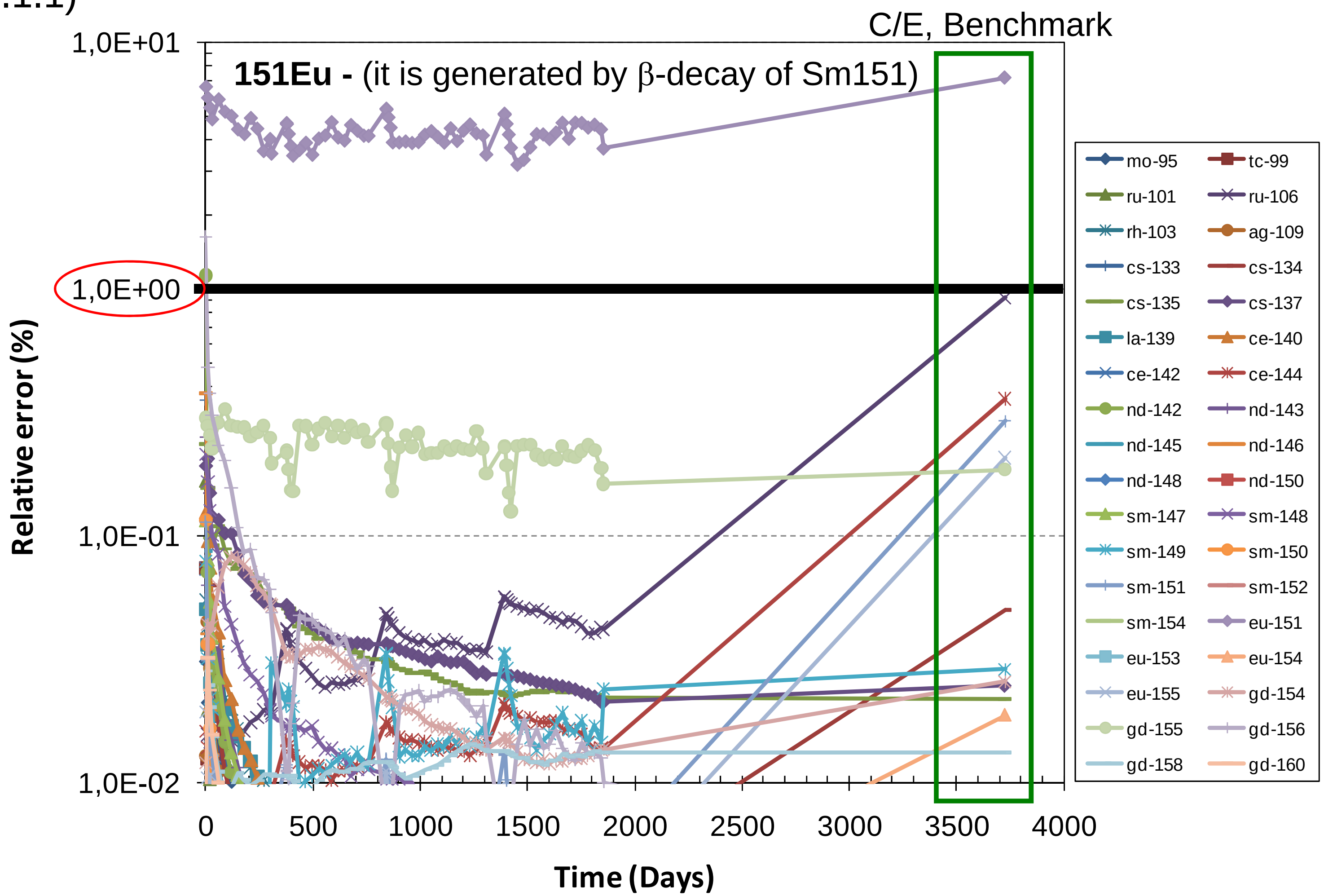
ΔN/N due to Fission Yields: FPs

- ΔN/N (%) predicted with Hybrid Monte Carlo Method due to **uncertainties in FYs** (JEFF-3.1.1)



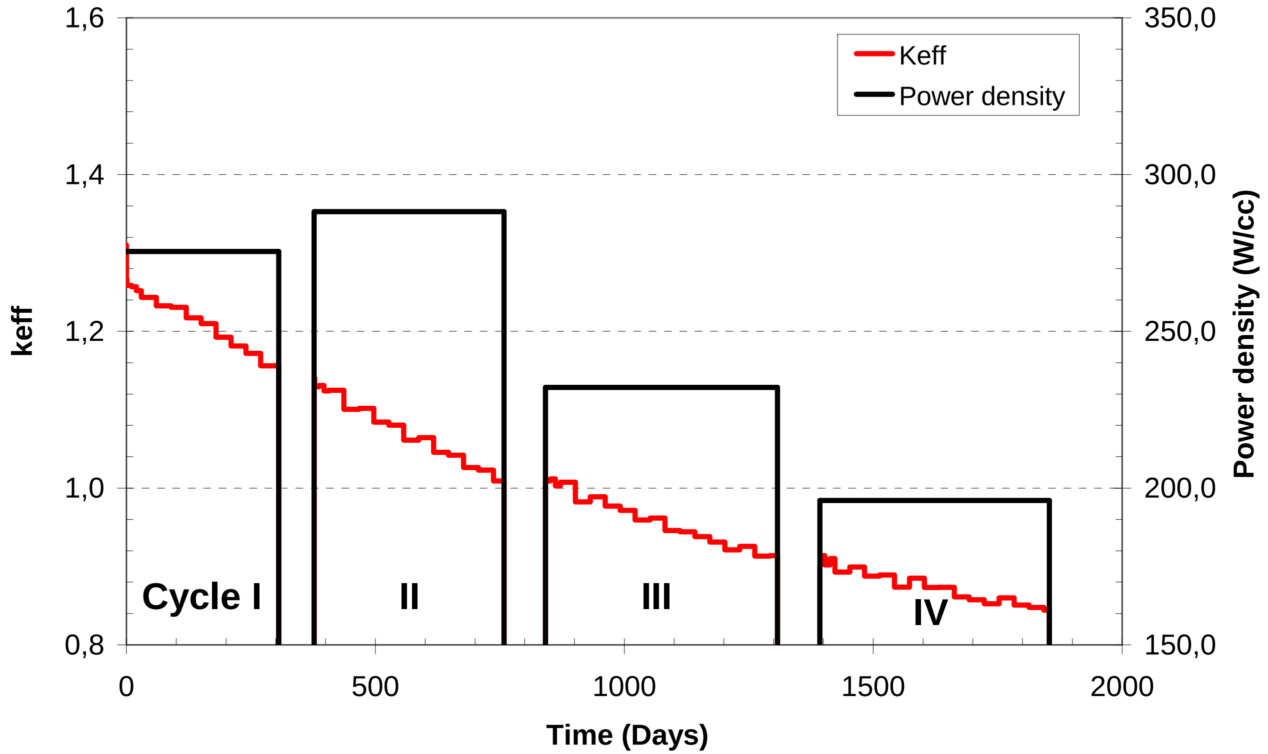
ΔN/N due to Decay Data: FPs

- ΔN/N (%) predicted with Hybrid Monte Carlo Method due to **uncertainties in Decay Data** (JEFF-3.1.1)



7. Criticality Uncertainty Analysis within "NEA/OECD UAM Project "

► Phase I-B Burnup: 4 cycles (case C). Burnup ~ 44 GWd/TMU

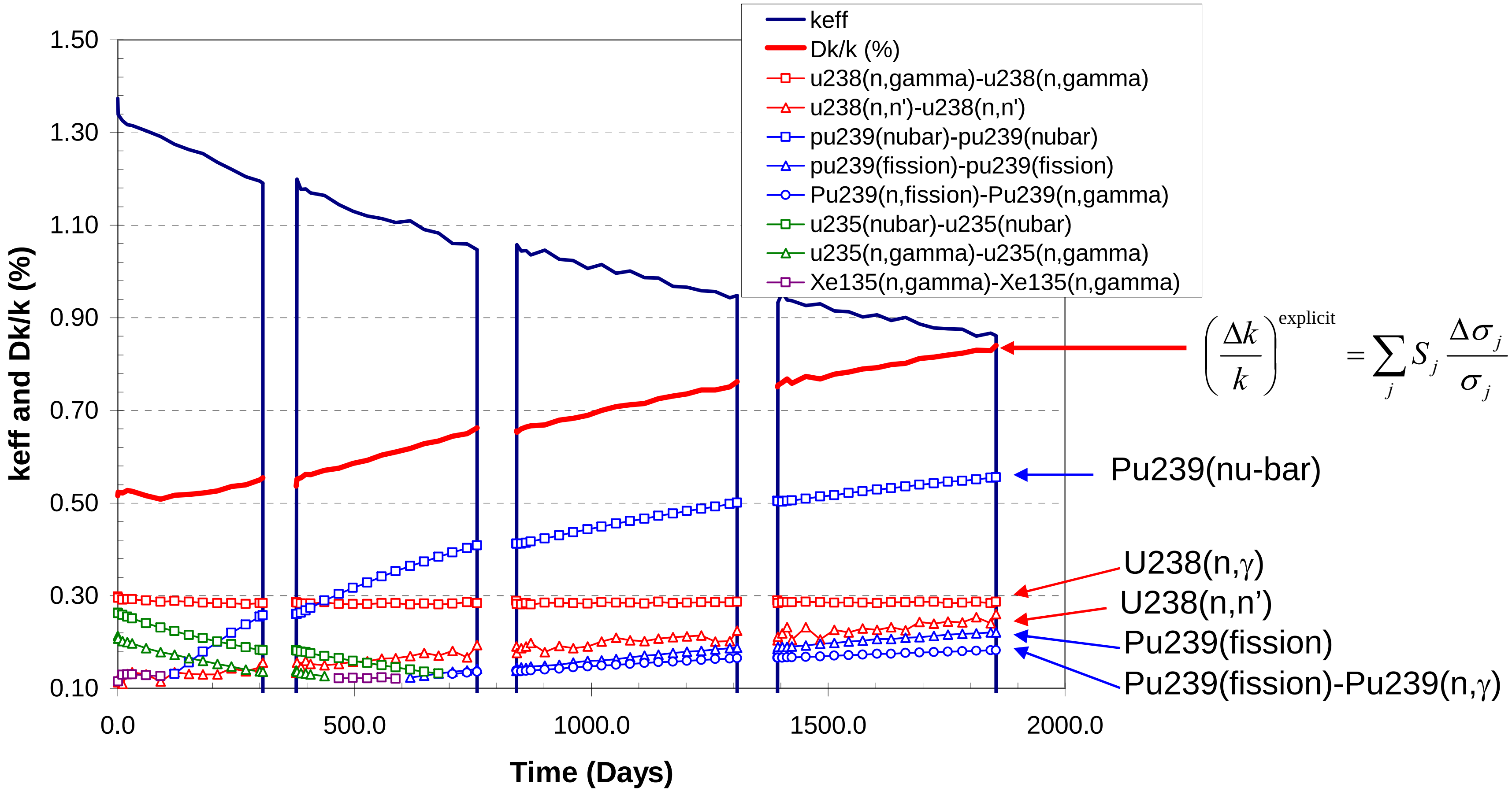


► Criticality Uncertainty Safety Analysis: "nuclear data uncertainties"

$$\frac{\Delta k}{k} = \sum_j S_j \frac{\Delta\sigma_j}{\sigma_j} + \sum_k \left[\frac{\Delta k / k}{\Delta N / N}\right]_k (\Delta N / N)_k$$

7.1 Prediction: $(\Delta k/k)^{expl}$ - SCALE/TSUNAMI

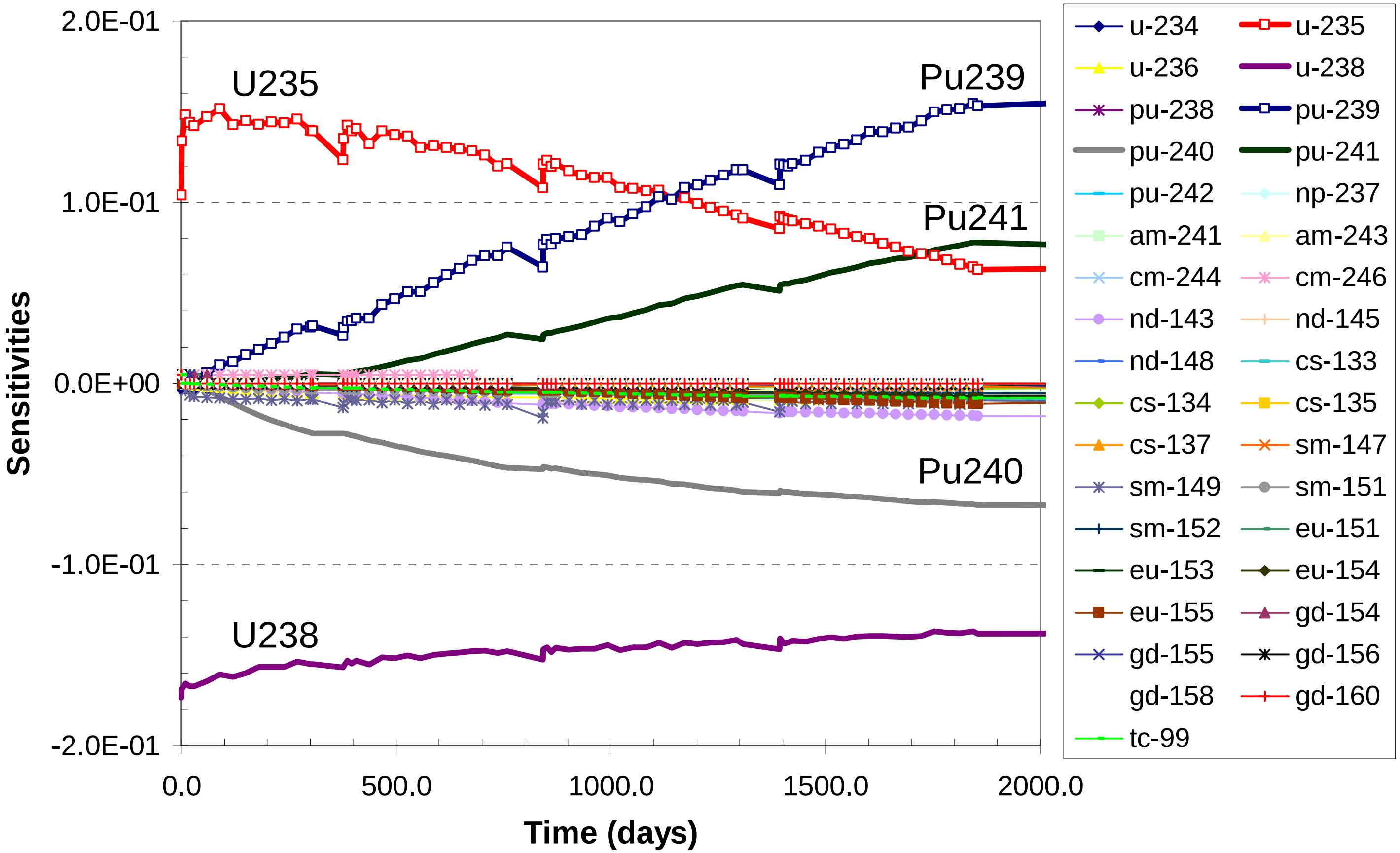
- Δk/k (%) predicted with SCALE6.0/TSUNAMI and the most important contributions
- In this figure, NO uncertainties in the isotopic inventory are taking into account!!



$$\left(\frac{\Delta k}{k}\right)^{\text{explicit}} = \sum_j S_j \frac{\Delta \sigma_j}{\sigma_j}$$

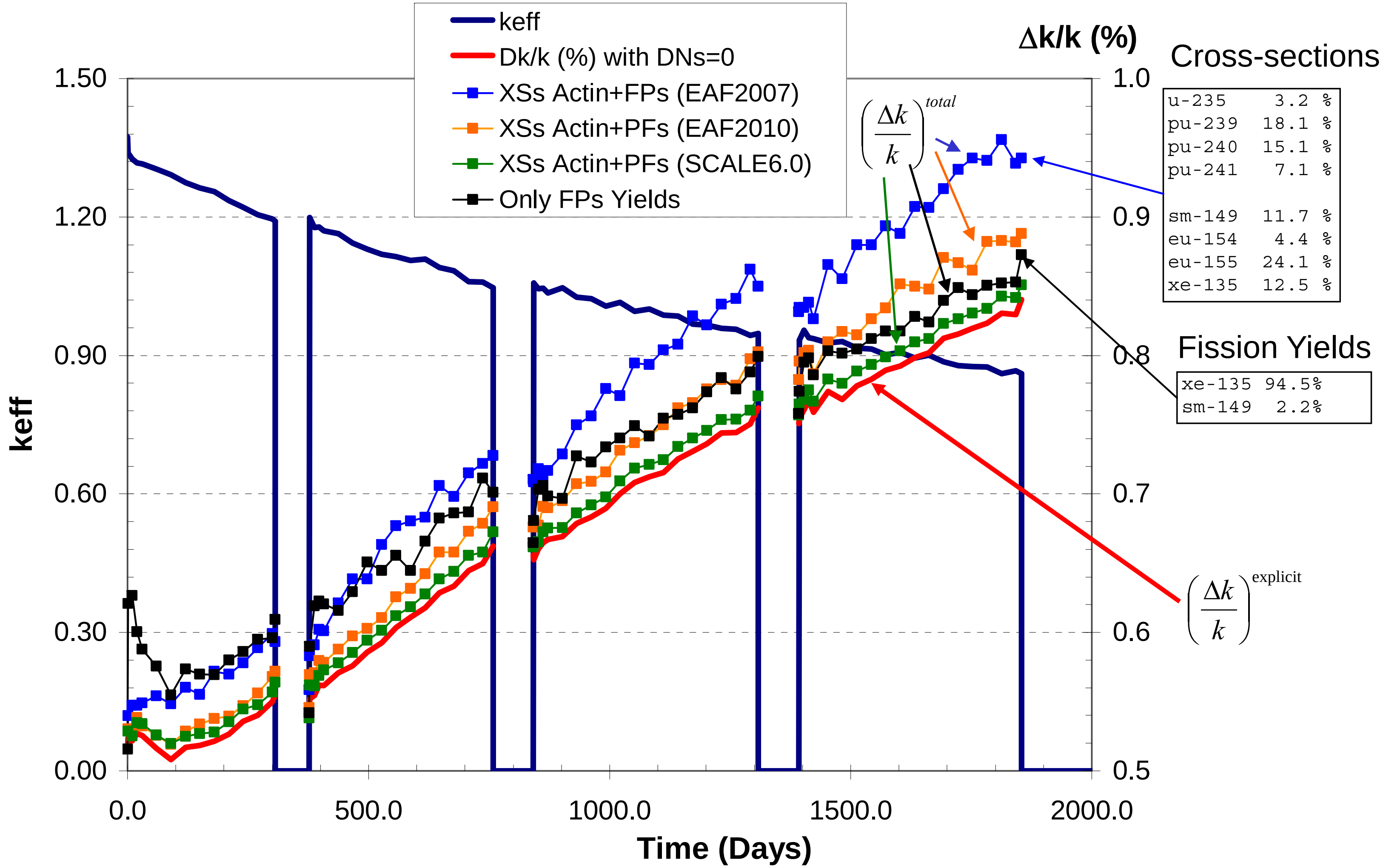
7.2 Sensitivities (Δk/k /ΔN/N): TSUNAMI

- Sensitivitye (Δk/k/ΔN/N) predicted with TSUNAMI (SCALE6.0) and the most important contributions by isotopes



7.3 Prediction of $(\Delta k/k)^{total}$ due to $\Delta N/N$

- Δk/k (%) due to the uncertainties in the isotopic inventory



8. Conclusions

We have carried out a ***Burnup Criticality Uncertainty Analysis*** for the Phase I-B -HFP Benchmark (Burnup ~ **44 GWd/TMU**)

1) Assuming **no uncertainties in the isotopic inventory**, TSUNAMI/SCALE6.0 predicts $\Delta k/k$ (%) at BOC:~ 0.5% and EOC :~ 0.8%

   At EOC, the most important reactions are: Pu239(nubar), U238(n,gamma), U238(n,n'), Pu239(fission) and Pu239(fission-capture)

2) To take into account **uncertainties in the isotopic inventory**, an Hybrid Monte-Carlo methodology that links transport and inventory calculations is presented

   It enables to estimate the impact of nuclear data (neutron cross section and fission yields) uncertainties on the inventory in transport-burnup combined problems.

   At EOC, we predict the values of $\Delta k/k$ (%) due to $\Delta N/N$:

   - **EAF2007/UN**: XSs for actinides:~ 0.3% and for fission products :~ 0.2%
     The most important isotopes:Pu239 and P240; Eu-155, Xe135 and Sm149
   - **EAF2010**: total uncertainty (ACTINIDES+FPS):~ 0.30%
   - **SCALE6.0**: total uncertainty (ACTINIDES+FPS):~ 0.15%
   - **Fission yields**: ~ 0.2%. The most important isotopes: Xe135
   - **Decay data:** negligible

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On going work…

In the framework of UAM/NEA group ("Uncertainy Analysis in Modelling"), we are discussing a Benchmark exercise (TMI-Pin cell) in order to compare different current **uncertainty burnup methodologies**:

- NRG/Total Monte Carlo
- AREVA/NUDUNA
- GRS/XSUSA
- UPM/Hybrid Monte Carlo
- …?¿

Results will be presented in the next UAM Meeting (UAM6) May 2012 in KIT (Germany)

Acknowledgments

Work performed in the framework of the agreement on "***Burnup Credit Criticality Safety"*** and "***Uncertainty Propagation in Criticality Calculations"*** between the Spanish Nuclear Safety Council (**CSN, Consejo de Seguridad Nuclear**) and the Polytechnical University of Madrid.